



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Sep 14, 2017 – 12:04 PM EDT

PDB ID : 5W0S  
EMDB ID: : EMD-8750  
Title : GroEL using cryoEM  
Authors : Roh, S.H.; Chiu, W.  
Deposited on : unknown  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

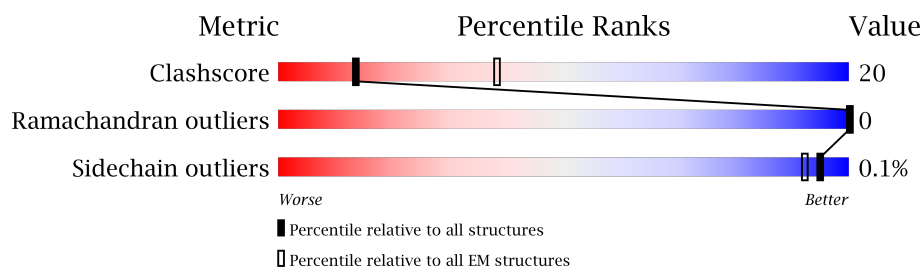
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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









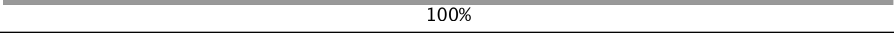
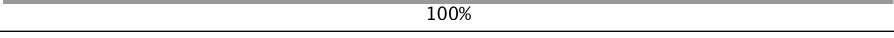
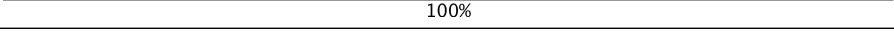
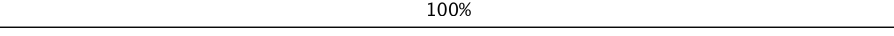
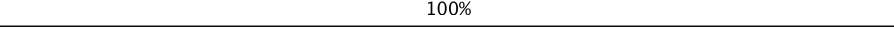
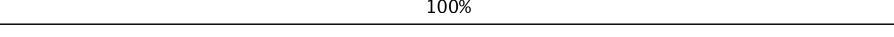
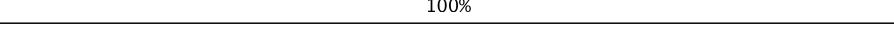
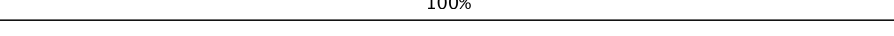
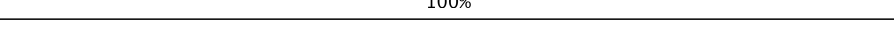
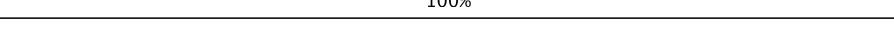
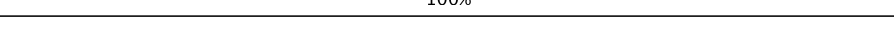
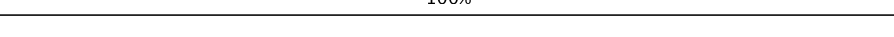
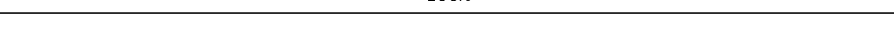






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	1-A	524	82% 18%
1	1-B	524	82% 18%
1	1-C	524	81% 19%
1	1-D	524	82% 18%
1	1-E	524	82% 18%
1	1-F	524	83% 17%
1	1-G	524	82% 18%
1	1-H	524	82% 18%
1	1-I	524	82% 18%

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Mol	Chain	Length	Quality of chain
1	1-J	524	 83% 17%
1	1-K	524	 81% 19%
1	1-L	524	 82% 18%
1	1-M	524	 82% 18%
1	1-N	524	 82% 18%
1	2-A	524	 52% 48%
1	2-B	524	 100%
1	2-C	524	 100%
1	2-D	524	 100%
1	2-E	524	 100%
1	2-F	524	 100%
1	2-G	524	 100%
1	2-H	524	 100%
1	2-I	524	 100%
1	2-J	524	 100%
1	2-K	524	 100%
1	2-L	524	 100%
1	2-M	524	 100%
1	2-N	524	 100%
1	3-A	524	 56% 43%
1	3-B	524	 100%
1	3-C	524	 100%
1	3-D	524	 100%
1	3-E	524	 100%
1	3-F	524	 100%

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Mol	Chain	Length	Quality of chain
1	3-G	524	100%
1	3-H	524	100%
1	3-I	524	100%
1	3-J	524	100%
1	3-K	524	100%
1	3-L	524	100%
1	3-M	524	100%
1	3-N	524	100%
1	4-A	524	61% 39%
1	4-B	524	100%
1	4-C	524	100%
1	4-D	524	100%
1	4-E	524	100%
1	4-F	524	100%
1	4-G	524	100%
1	4-H	524	100%
1	4-I	524	100%
1	4-J	524	100%
1	4-K	524	100%
1	4-L	524	100%
1	4-M	524	100%
1	4-N	524	100%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 65574 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	2-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	3-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	4-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-B	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-C	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-D	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-E	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-F	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-G	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-H	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-I	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-J	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-K	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-L	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-M	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-N	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	conflict	UNP Q6Q099
B	13	GLY	ARG	conflict	UNP Q6Q099
C	13	GLY	ARG	conflict	UNP Q6Q099
D	13	GLY	ARG	conflict	UNP Q6Q099
E	13	GLY	ARG	conflict	UNP Q6Q099
F	13	GLY	ARG	conflict	UNP Q6Q099
G	13	GLY	ARG	conflict	UNP Q6Q099
H	13	GLY	ARG	conflict	UNP Q6Q099
I	13	GLY	ARG	conflict	UNP Q6Q099
J	13	GLY	ARG	conflict	UNP Q6Q099
K	13	GLY	ARG	conflict	UNP Q6Q099
L	13	GLY	ARG	conflict	UNP Q6Q099
M	13	GLY	ARG	conflict	UNP Q6Q099
N	13	GLY	ARG	conflict	UNP Q6Q099

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	AltConf
2	1-A	19	Total O 19 19	0
2	1-B	12	Total O 12 12	0
2	1-C	14	Total O 14 14	0
2	1-D	14	Total O 14 14	0
2	1-E	10	Total O 10 10	0
2	1-F	6	Total O 6 6	0
2	1-G	13	Total O 13 13	0
2	1-H	1	Total O 1 1	0
2	1-I	3	Total O 3 3	0
2	1-J	5	Total O 5 5	0
2	1-K	1	Total O 1 1	0
2	1-L	2	Total O 2 2	0

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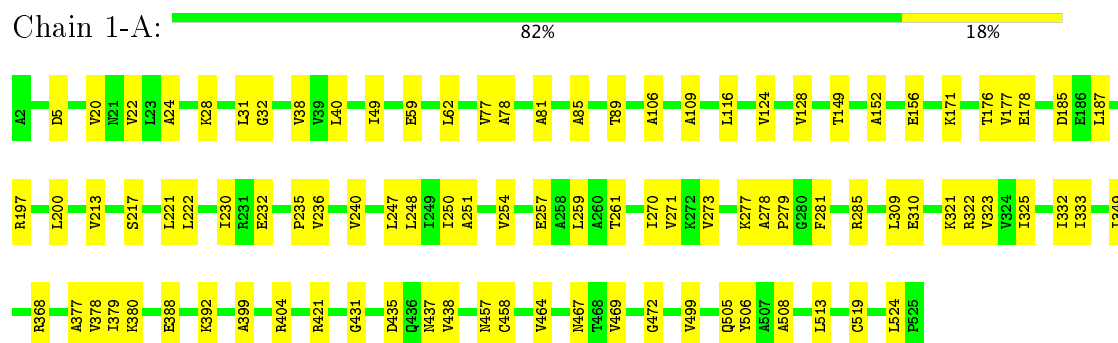
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Mol	Chain	Residues	Atoms		AltConf
2	1-M	5	Total	O	0
			5	5	
2	1-N	2	Total	O	0
			2	2	

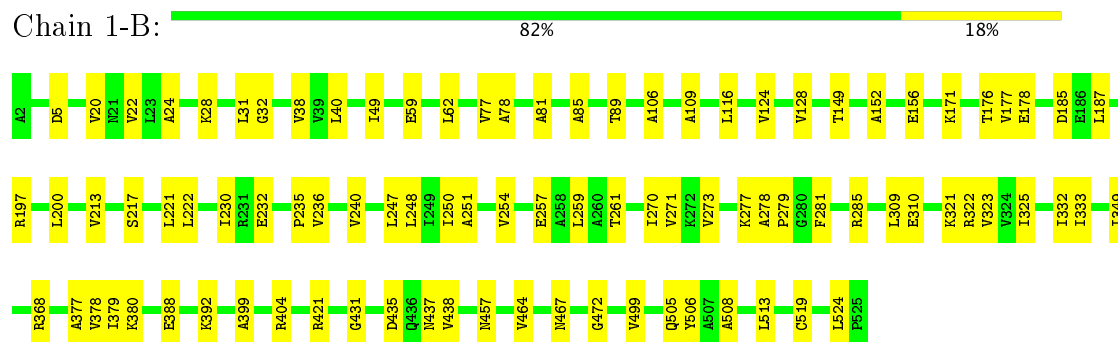
### 3 Residue-property plots

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

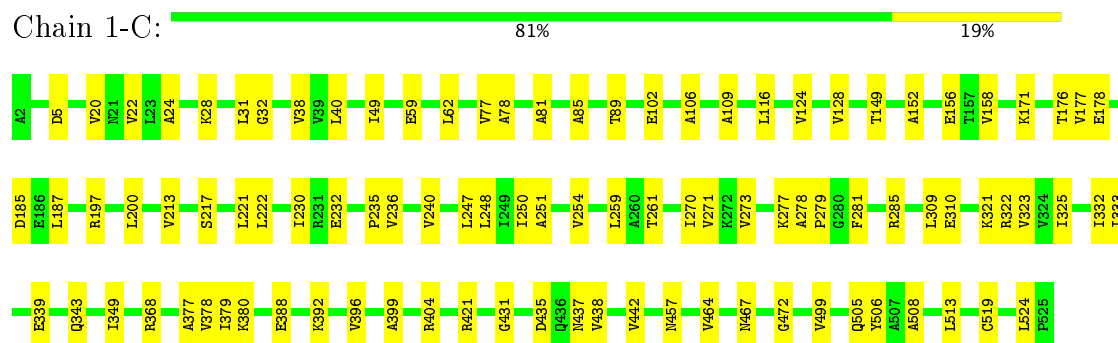
- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin

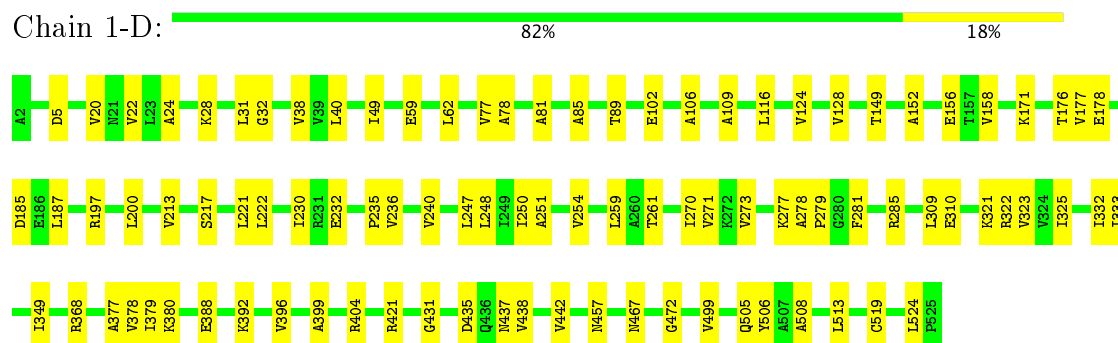


- Molecule 1: 60 kDa chaperonin

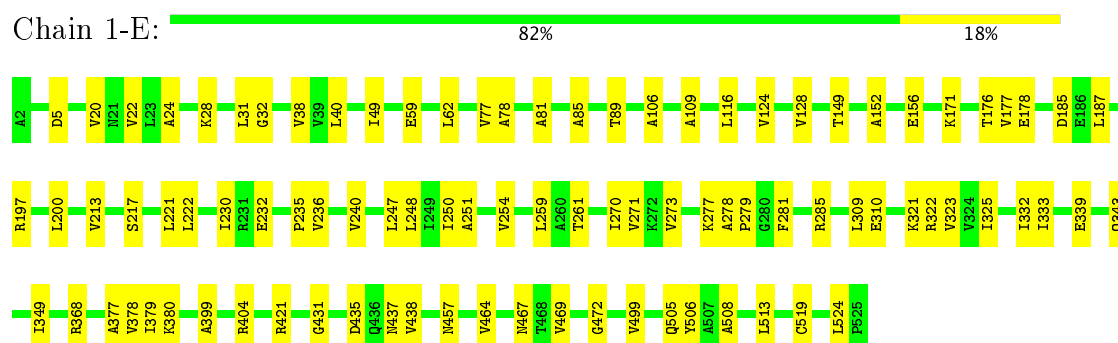


- Molecule 1: 60 kDa chaperonin

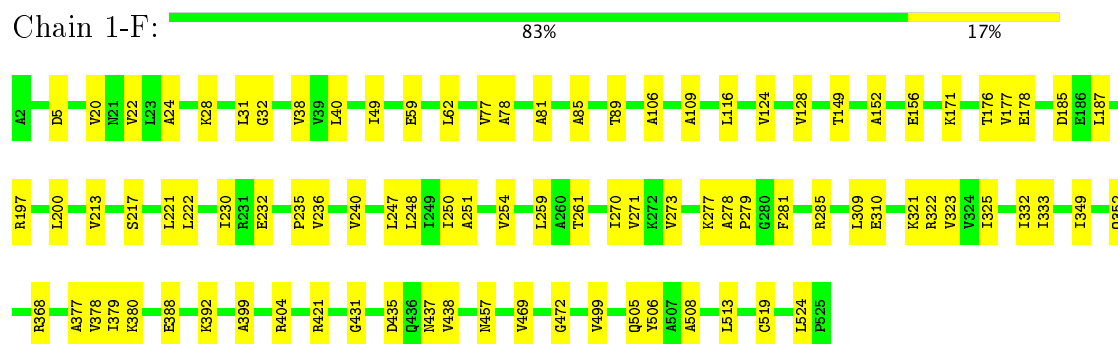




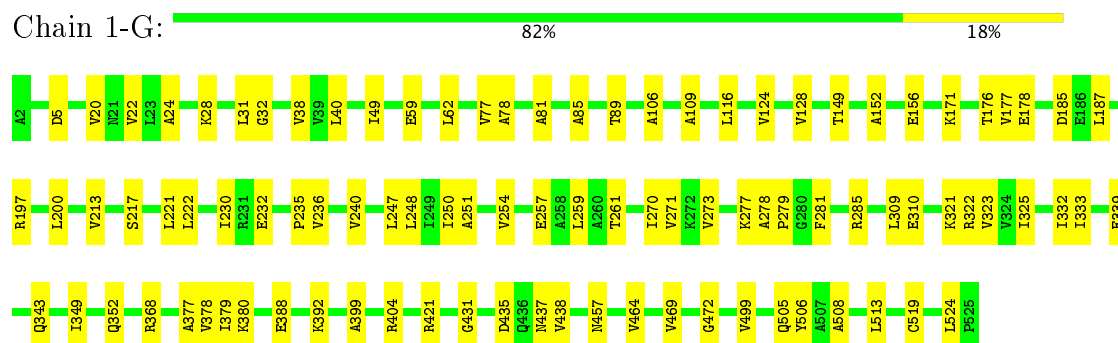
- Molecule 1: 60 kDa chaperonin



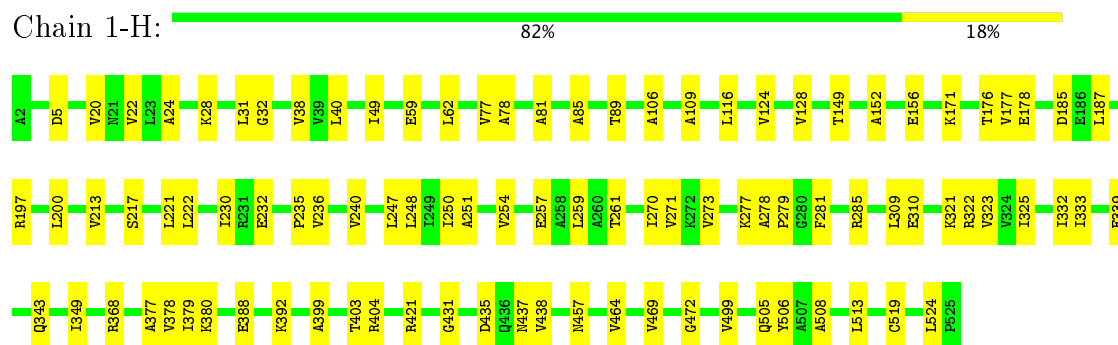
- Molecule 1: 60 kDa chaperonin



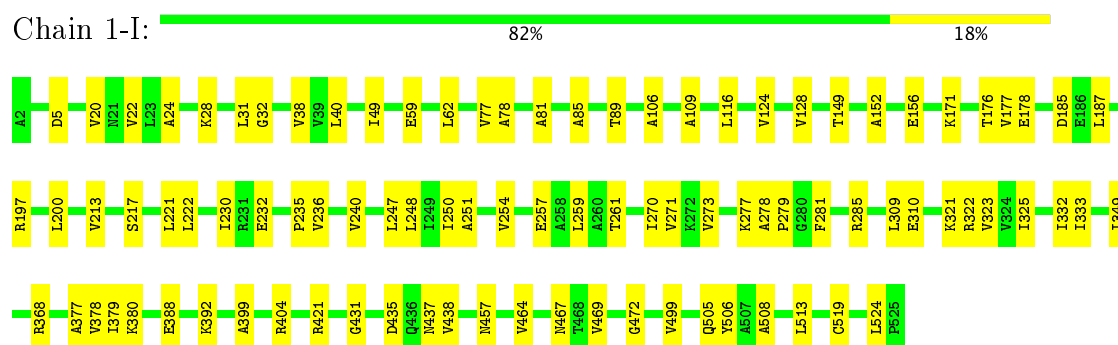
- Molecule 1: 60 kDa chaperonin



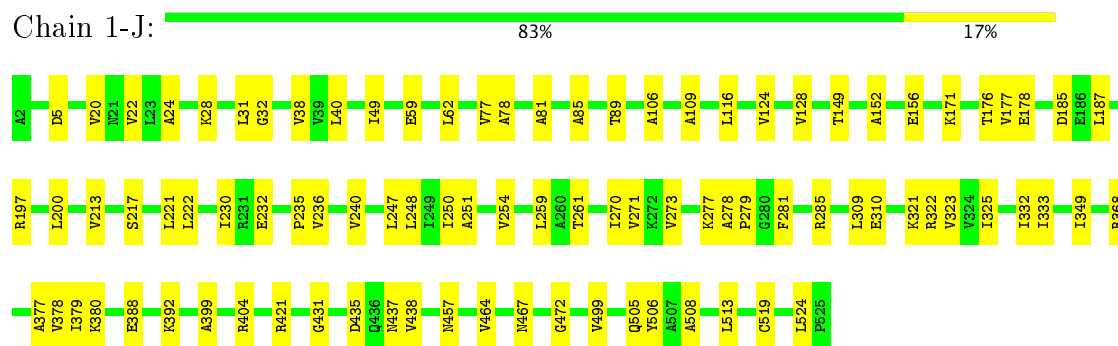
- Molecule 1: 60 kDa chaperonin



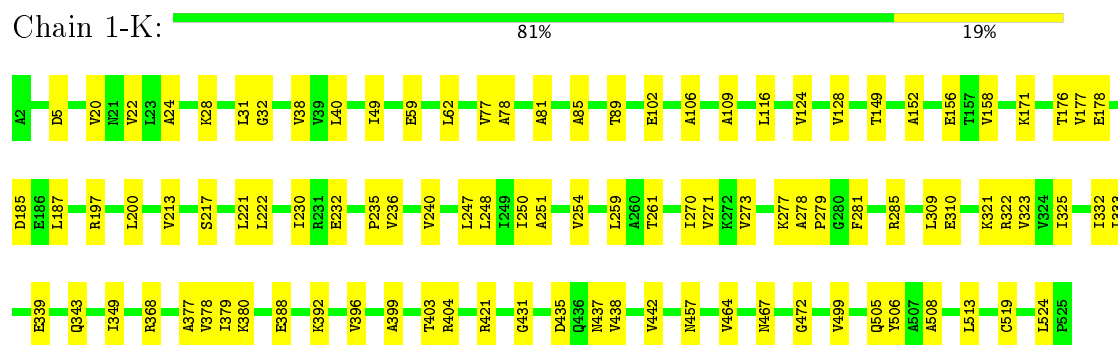
- Molecule 1: 60 kDa chaperonin



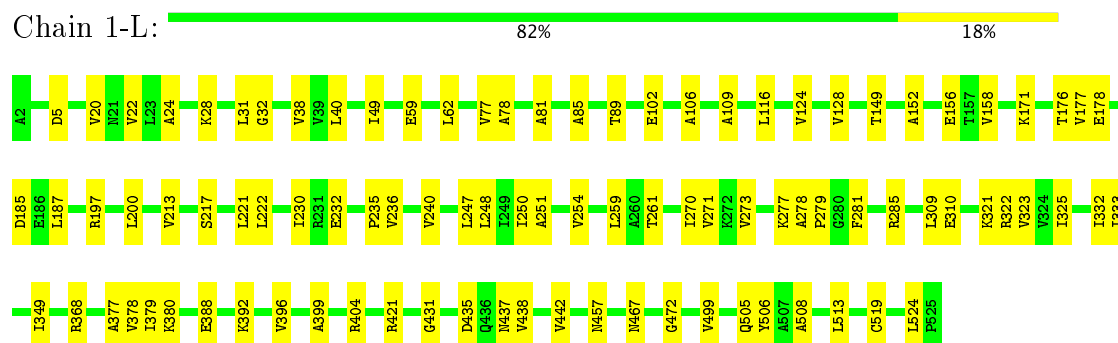
- Molecule 1: 60 kDa chaperonin



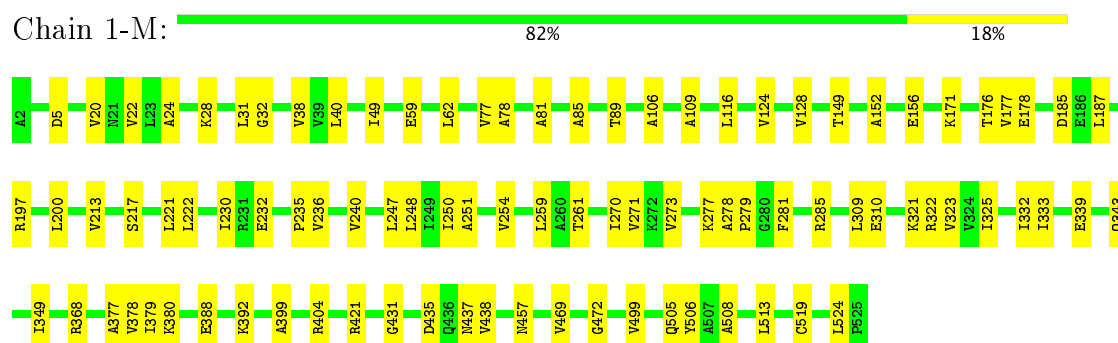
- Molecule 1: 60 kDa chaperonin



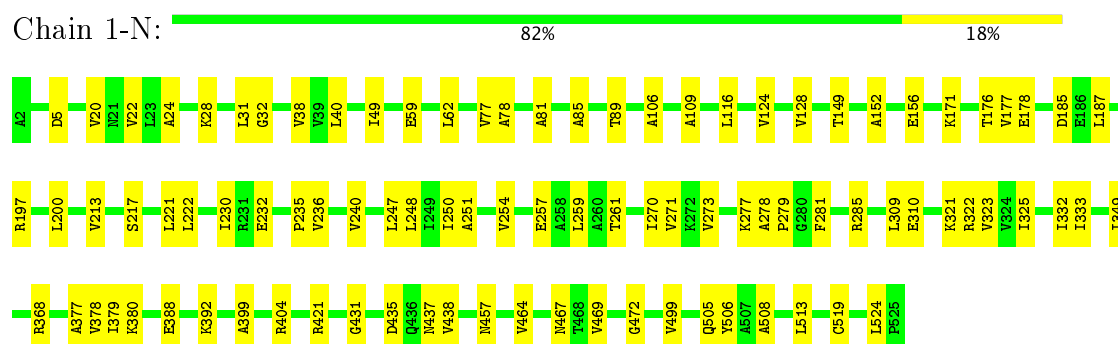
- Molecule 1: 60 kDa chaperonin



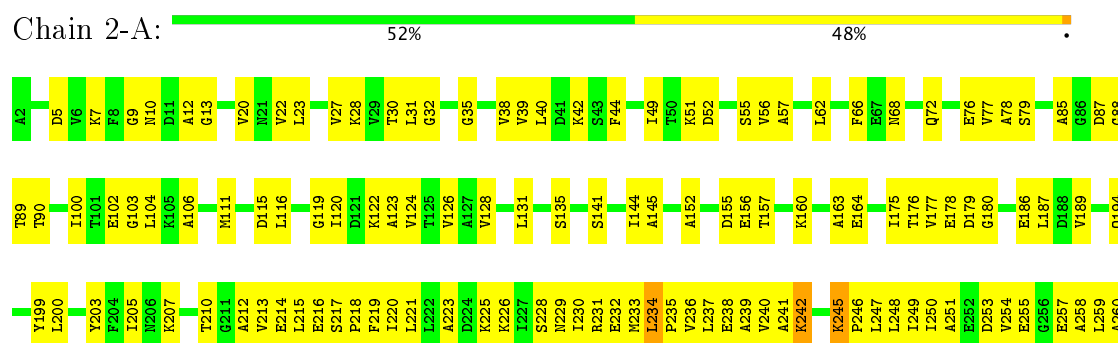
- Molecule 1: 60 kDa chaperonin



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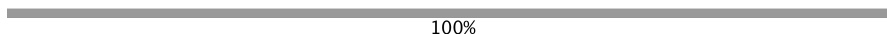




THR	VAL	ARG	SER	LYS	GLY	LYS
GLU	GLU	GLU	GLU	ALA	LEU	ALA
GLU	SER	LYS	GLU	GLY	GLN	VAL
TYR	LYS	LEU	ILE	LYS	ASP	THR
GLY	LEU	GLN	GLY	PRO	GLU	ALA
ASN	ALA	GLU	MET	LEU	LEU	ALA
MET	ASP	ARG	GLU	LEU	ASP	VAL
ILE	LEU	VAL	LEU	ILE	VAL	GLU
GLU	ARG	ALA	GLU	ILE	VAL	GLU
MET	GLY	LYS	GLY	ALA	GLY	LYS
ILE	ASN	ALA	THR	ASP	MET	ALA
LEU	GLU	GLY	LEU	VAL	GLN	LEU
VAL	ASP	GLY	GLU	GLU	PHE	SER
PRO	GLN	VAL	ASP	GLY	ASP	SER
THR	ASN	ALA	LEU	ARG	PRO	LYS
LYS	VAL	VAL	GLY	ALA	GLY	LYS
VAL	ARG	ILE	LYS	ALA	TYR	ILE
LEU	LEU	ALA	THR	ASN	PHE	ALA
GLN	ARG	THR	ILE	ASN	ILE	ALA
TYR	ALA	GLU	ASN	THR	ASN	GLN
ALA	MET	VAL	LYS	MET	LYS	VAL
ALA	GLU	GLU	ASP	ARG	PRO	GLY
SER	ALA	MET	THR	GLY	GLU	THR
VAL	PRO	LYS	THR	ILE	THR	ILE
ALA	LEU	GLU	THR	VAL	GLY	SER
GLY	GLN	LYS	ILE	LYS	ALA	ASN
LEU	ARG	LYS	ILE	VAL	VAL	ASN
GLU	GLN	THR	ILE	THR	VAL	GLN
GLU	CYS	GLU	GLU	ALA	PRO	VAL
CYS	GLY	ALA	GLU	PRO	PHE	GLY
MET	GLU	LEU	ALA	GLY	ILE	LYS
VAL	GLU	HIS	ALA	PHE	LEU	LEU
THR	PRO	ALA	ILE	GLY	LEU	ILE
ASP	SER	THR	GLN	ASP	ALA	ALA
PRO	VAL	ARG	GLY	ARG	ASP	GLU
	ALA	ALA	VAL	LYS	LYS	ALA
	ASN	VAL	ALA	ALA	ILE	ASP
	THR	GLU	GLN	MET	SER	LYS
	VAL	GLU	ILE	LEU	ASN	VAL
	LYS	GLY	ARG	GLN	ILE	GLY
	GLY	VAL	GLN	ILE	ARG	LYS
	ASP	ALA	ILE	THR	MET	GLY
	ASN	GLY	GLU	THR	LEU	VAL
	TYR	GLY	ALA	LEU	PRO	ILE
	THR	VAL	THR	THR	VAL	THR
	TYR	ALA	SER	GLY	GLU	VAL
	ASN	LEU	ASP	THR	ALA	ASP
	ALA	ARG	TYR	ILE	VAL	THR

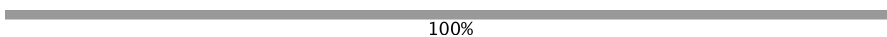
- Molecule 1: 60 kDa chaperonin

Chain 2-D:

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 2-E:



[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 2-F:  100%

[illegible]

THR GLU GLU TYR GLY ASN MET ILE ASP MET GLY ILE LEU ASP PRO THR LYS VAL THR ARG SER LEU GLN TYR ALA ALA VAL ALA GLY LEU MET ILE THR THR GLU CYS MET VAL THR ASP LEU PRO

- Molecule 1: 60 kDa chaperonin

Chain 2-G:  100%

ALA	ALA	ALA	LYS	ASP	VAL	LYS	PHE	GLY	GLY	ASN	ASP	ALA	GLY	VAL	VAL	LYS	NET	LEU	ARG	GLY	VAL	ASN	VAL	VAL	LEU	ALA	ASP	ALA	VAL	LYS	VAL	THR	THR	LEU	GLY	GLY	PRO	LYS	GLY	ARG	ASN	VAL	VAL	VAL	LEU	LEU	ASP	LYS	LYS	SER	PHE	GLY	GLY	ALA	ALA	PRO	THR	THR	LYS	ASP	GLY	VAL	SER	VAL	ALA	ALA	ARG	GLU	ILE
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LYS	ALA	VAL	THR	VAL	ALA	VAL	GLU	GLU	LEU	LYS	ALA	LEU	SER	VAL	SER	PRO	CYS	SER	ASP	SER	LYS	ALA	ALA	ILE	ALA	ALA	GLN	GLY	THR	THR	ILE	SER	SER	ALA	ASN	SER	SER	ASP	GLU	THR	VAL	GLY	GLY	LYS	LYS	LEU	ILE	ALA	ALA	GLU	ALA	ALA	ASP	MET	ASP	LYS	VAL	GLY	LYS	GLU	GLY	VAL	GLY	ILE	THR	VAL	GLU	ASP	GLY
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GLY	LEU	GLN	ASP	GLU	LEU	ASP	VAL	VAL	GLU	GLY	MET	GLN	PHE	ASP	ARG	TYR	LEU	SER	PRO	TYR	PHE	ILE	ASN	LYS	PRO	GLU	THR	GLY	ALA	VAL	GLU	LEU	SER	GLU	PRO	PHE	ILE	LEU	LEU	ALA	ASP	LYS	ILE	SER	ASN	ARG	GLU	MET	LEU	PRO	VAL	LEU	GLU	ALA	VAL
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LYS	ALA	GLY	LYS	PRO	LEU	LEU	ILE	ILE	ALA	GLU	ASP	VAL	GLU	GLY	GLU	ALA	GLU	ALA	LEU	ALA	THR	LEU	VAL	VAL	ASN	THR	THR	MET	ARG	GLY	ILE	VAL	LYS	VAL	VAL	ALA	ALA	ALA	VAL	LYS	LYS	ALA	ALA	ALA	ALA	GLY	GLY	PHE	ASP	GLY	ASP	ARG	ARG	ARG	LYS	ALA	ALA	ALA	GLN	ASP	LEU	ILE	ALA	ALA	THR	THR	GLY	GLY	THR	VAL
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SER	GLU	GLU	ILE	GLY	MET	GLU	LEU	LYS	ALA	THR	LEU	GLU	ASP	LEU	GLY	GLN	ALA	LYS	ARG	VAL	VAL	ILE	VAL	ASN	LYS	ASP	THR	THR	THR	ILE	ILE	ASP	GLY	VAL	GLY	GLY	GLU	GLU	ALA	ALA	ALA	ILE	GLN	GLY	ARG	VAL	VAL	GLN	ILE	THR	THR	THR	ASP	SER	THR
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ARG	GLY	LEU	GLN	GLU	ARG	VAL	ALA	LYS	LEU	ALA	GLY	GLY	VAL	ALA	VAL	ILE	LYS	VAL	GLY	ALA	ALA	LYS	GLU	THR	GLU	GLU	VAL	GLU	MET	LYS	GLU	LYS	LYS	ALA	ARG	VAL	GLU	ASP	LEU	HIS	ALA	ALA	THR	ARG	ALA	VAL	VAL	GLU	GLY	VAL	VAL	VAL	VAL	GLY	GLY	VAL	ALA	LEU	ILE
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VAL	ALA	SER	LYS	LEU	ALA	ASP	LEU	ARG	GLY	GLN	ASN	GLU	GLN	ASN	VAL	GLY	ILE	LYS	VAL	LEU	ARG	ALA	ALA	MET	GLU	GLU	ARG	PRO	LEU	GLN	ILE	VAL	VAL	ASN	CYS	GLY	GLU	GLU	PRO	SER	VAL	VAL	ALA	ALA	ASN	THR	VAL	LYS	GLY	GLY	ASP	GLY	ASN	TYR	TYR	ASN	ALA
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THR	GLU	GLU	GLY	ASN	MET	ILE	ASP	MET	GLY	ILE	LEU	ASP	PRO	THR	LYS	VAL	THR	ARG	SER	ALA	LEU	GLN	TYR	ALA	ALA	SER	VAL	ALA	GLY	LEU	MET	ILE	THR	THR	GLU	CYS	MET	MET	VAL	THR	ASP	LEU	PRO
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- Molecule 1: 60 kDa chaperonin

Chain 2-H:  100%

ALA ALA ALA LYS ASP VAL LYS PHE GLY ASN ASP ALA GLY VAL LYS MET MET LEU ARG GLY VAL ASN VAL VAL LEU ASP ALA ALA VAL LYS VAL VAL THR THR LEU GLY PRO PRO GLY GLY ARG ASN VAL VAL VAL LEU LEU ASP LYS LYS SER PHE GLY ALA PRO THR THR LYS ASP GLY VAL SER VAL ALA ARG GLU ILE

LEU	GLU	ASP	LYS	PHS	GLU	ASN	MET	GLY	ALA	ALA	GLN	VAL	VAL	GLU	GLU	VAL	ALA	ALA	SER	LYS	ALA	ASN	ASP	ASP	ALA	ALA	GLY	GLY	THR	THR	THR	ALA	THR	VAL	LEU	ALA	GLN	ALA	ILE	ILE	THR	THR	GLU	GLY	LEU	LYS	ALA	VAL	VAL	ALA	ALA	ALA	GLY	MET	ASN	PRO	MET	ASP	LYS	ARG	GLY	ILE
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LYS	ALA	VAL	THR	VAL	ALA	VAL	GLU	GLU	LEU	LYS	ALA	LEU	SER	VAL	PRO	CYS	CYS	SER	ASP	SER	LYS	ALA	ALA	ILE	ALA	GLN	GLY	THR	ILE	SER	ALA	ASN	SER	ASP	GLU	THR	VAL	GLY	LYS	ILE	ILE	ALA	GLU	ALA	MET	ASP	LYS	VAL	GLY	LYS	GLU	GLY	VAL	ILE	THR	VAL	GLU	ASP	GLY	THR
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GLY	LEU	GLN	ASP	GLU	LEU	ASP	VAL	GLU	GLY	GLN	PHE	ASP	ARG	GLY	TYR	LEU	SER	PRO	TYR	THR	ILE	ALA	VAL	GLU	LEU	GLU	SER	PRO	PHE	ILE	LEU	LEU	ALA	ASP	LYS	LYS	ILE	ILE	SER	ASN	ILE	ARG	GLU	GLU	LEU	LEU	PRO	VAL	GLU	ALA	VAL
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LYS ALA LYS GLY LYS PRO LEU LEU ILE ILE ALA ALA GLU ASP VAL VAL GLU GLY GLU GLU ALA ALA ASN THR MET ARG GLY ILE VAL VAL LYS LYS VAL VAL ALA ALA VAL VAL LYS LYS PRO PHE GLY GLY GLY ASP ARG ARG LYS ALA ALA MET LEU LEU GLN ASP ILE ILE ALA ALA THR LEU THR GLY GLY THR VAL

[illegible]

ARG	GLY	LYS	LEU	GLN	GLU	ARG	VAL	ALA	LYS	LEU	ALA	GLY	GLY	VAL	ALA	VAL	ILE	LYS	VAL	GLY	ALA	ALA	LYS	LYS	LYS	GLU	LYS	ALA	ARG	ARG	VAL	VAL	GLU	GLY	VAL	VAL	ALA	ALA	GLY	GLY	VAL	ALA	ALA	LEU	ILE	ARG
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VAL	ALA	SER	LYS	LEU	ALA	ASP	LEU	ARG	GLY	GLN	ASN	GLU	GLY	ILE	LYS	VAL	ALA	LEU	ARG	ALA	MET	GLU	ALA	ALA	PRO	LEU	ARG	GLN	ILE	VAL	VAL	ASN	CYS	GLY	GLU	GLU	PRO	SER	VAL	VAL	ALA	ALA	ASN	THR	VAL	LYS	GLY	GLY	ASP	GLY	ASN	TYR	TYR	ASN	ALA	ALA
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THR  
THR  
GLU  
CYS  
MET  
VAL  
THR  
ASP  
LEU  
PRO

- Molecule 1: 60 kDa chaperonin

Chain 2-I:  100%

[illegible]

LEU GLU ASP LYS PHE GLU ASN MET MET GLY GLY ALA ALA GLN MET VAL LYS GLU VAL VAL SER LYS ALA LYS ASN ASP ALA ALA GLY ASP GLY THR THR THR ALA THR VAL LEU VAL ALA ALA GIN ALA ALA ILE ILE THR THR GLY LEU LYS ALA VAL VAL ALA ALA GLY MET ASN PRO MET ASP LEU LYS ARG GLY ILE ILE

LYS	ALA	VAL	THR	VAL	ALA	VAL	GLU	GLU	LEU	LYS	ALA	LEU	VAL	SER	PRO	CYS	SER	ASP	SER	LYS	ALA	ILE	ALA	GLN	VAL	GLY	THR	ILE	SER	ASN	SER	ASP	GLU	THR	VAL	GLY	LYS	LEU	ILE	ALA	GLU	ALA	NET	ASP	LYS	VAL	GLY	GLU	ILE	THR	VAL	GLU	ASP	GLY	THR
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LYS	ALA	GLY	LYS	PRO	LEU	ILE	ALA	GLU	ASP	VAL	GLU	GLY	GLU	ALA	ALA	LEU	ALA	THR	LEU	VAL	VAL	ASN	THR	MET	ARG	GLY	ILE	VAL	LYS	LYS	VAL	ALA	ALA	ALA	VAL	LYS	ALA	ALA	PRO	PHE	GLY	GLY	GLY	ASP	ARG	ARG	LYS	LEU	ALA	ALA	MET	LEU	GLN	ASP	ILE	ALA	ALA	THR	LEU	THR	GLY	GLY	THR	THR	VAL
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SER	GLU	GLU	ILE	GLY	GLU	GLU	GLU	LYS	ALA	THR	LEU	GLU	ASP	GLY	GLY	GLN	ALA	LYS	ARG	VAL	VAL	ILE	ASN	LYS	ASP	THR	THR	THR	ILE	ILE	ASP	GLY	VAL	GLY	GLU	GLU	ALA	ALA	ILE	GLN	GLY	ARG	VAL	VAL	GLN	GLN	ILE	ILE	THR	SER	ASP	TYS	THR
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ARG	GLY	LEU	GLN	GLU	ARG	VAL	ALA	LYS	LEU	ALA	GLY	GLY	VAL	ALA	ILE	LYS	THR	GLU	GLU	VAL	MET	LYS	GLU	LYS	LYS	ALA	ARG	VAL	GLU	ASP	ALA	LEU	HIS	ALA	THR	ANG	ALA	VAL	VAL	GLU	GLY	GLY	VAL	ALA	ILE	PAC
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VAL	ALA	SER	LYS	LEU	ALA	ASP	LEU	ARG	GLY	GLN	ASN	GLU	ASP	GLN	ASN	VAL	VAL	GLY	TYR	LYS	ASN	ASP	GLY	GLY	GLY	GLY	TYR	TYR	ASN	ALA	ALA
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THR	GLU	GLU	TYR	GLY	ASN	MET	ILE	ASP	MET	GLY	ILE	LEU	ASP	PRO	THR	LYS	VAL	THR	ARG	SER	ALA	LEU	GLN	TYR	ALA	ALA	SER	VAL	ALA	GLY	LEU	MET	ILE	THR	THR	GLU	CYS	MET	VAL	THR	ASP	LEU	PRO
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- Molecule 1: 60 kDa chaperonin

Chain 2-J:  100%

ALA  
ALA  
LYS  
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LYS  
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ASN  
ASP  
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[illegible]

LYS	ALA	VAL	THR	VAL	ALA	VAL	GLU	GLU	LEU	LYS	ALA	LEU	SER	ASP	SER	LYS	ALA	ILE	ALA	GLN	GLY	THR	ILE	SER	ASN	SER	ASP	GLU	THR	VAL	GLY	LYS	ILE	ALA	ALA	MET	ASP	LYS	VAL	GLY	LYS	GLU	GLY	VAL	ILE	THR	VAL	GLU	ASP	GLY
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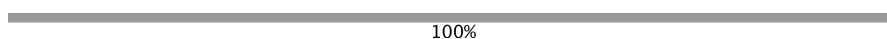
GLY LEU GLN ASP ASP VAL VAL GLU GLY MET GIN PHE ASP ARG TYR LEU SER PRO TYR PHE ILE ASN LYS PRD THR GLY ALA VAL GLU LEU GLU SER PRO PHE ILE LEU LEU LEU ALA ASP LYS LYS ILE ILE SER ASN ILE ARG GLU MET LEU PRO VAL LEU GLU ALA VAL



THR	VAL	ARG	SER	LYS
GLU	ALA	GLU	GLU	ALA
GLU	SER	LYS	GLU	GLY
TYR	LYS	LEU	ILE	LYS
GLY	LEU	GLN	GLY	PRO
ASN	ALA	GLU	MET	LEU
MET	ASP	ARG	GLU	LEU
ILE	LEU	VAL	LEU	ILE
ASP	ARG	VAL	GLU	ILE
MET	GLY	LYS	LYS	ALA
GLY	GLN	LEU	ALA	GLU
ILE	ASN	LEU	THR	ASP
LEU	GLU	GLY	LEU	VAL
ASP	ASP	GLY	GLU	GLY
PRO	GLN	VAL	ASP	GLY
THR	ASN	ALA	LEU	GLU
LYS	VAL	VAL	GLY	ALA
VAL	GLY	ILE	GLN	LEU
THR	ILE	LYS	ALA	ALA
ARG	LYS	VAL	LYS	THR
SER	VAL	GLY	ARG	LEU
ALA	ALA	ALA	VAL	VAL
LEU	LEU	ALA	VAL	VAL
GLN	ARG	THR	ILE	ASN
TYR	ALA	GLU	ASN	THR
ALA	MET	VAL	LYS	MET
ALA	ALA	GLU	ASP	ARG
SER	SER	ALA	MET	GLY
VAL	PRO	LYS	THR	ILE
ALA	LEU	GLU	THR	VAL
GLY	ARG	LYS	ILE	LYS
ILE	GLN	LYS	ILE	VAL
ILE	ILE	ALA	ASP	ALA
THR	VAL	ARG	GLY	ALA
THR	LEU	VAL	VAL	VAL
THR	ASN	GLU	GLY	LYS
GLU	CYS	ASP	GLU	ALA
THR	GLY	ALA	GLU	ALA
CYS	GLY	LEU	ALA	PRO
MET	MET	LEU	ALA	GLY
VAL	GLU	HIS	ALA	GLY
THR	PRO	ALA	ILE	PHE
THR	THR	THR	ALA	GLY
ASP	SER	THR	GLN	ASP
LEU	VAL	ARG	GLY	ARG
PRO	VAL	ALA	ARG	ARG
	ALA	ALA	VAL	LYS
	ASN	VAL	ALA	LYS
	THR	GLU	GLN	MET
	VAL	GLY	ILE	LEU
	LYS	GLY	ARG	GLN
	GLY	VAL	GLN	ASP
	ASP	ALA	ILE	ALA
	ASN	GLY	GLU	THR
	TYR	GLY	GLU	LEU
	THR	GLY	ALA	THR
	TYR	VAL	THR	GLY
	TYR	ALA	SER	GLY
	ASN	LEU	ASP	THR
	ALA	ILE	TYR	THR
	ALA	ARG	ASP	ILE

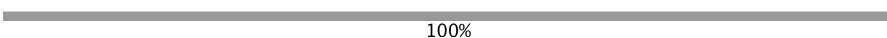
- Molecule 1: 60 kDa chaperonin

Chain 2-K:

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 2-L:

[illegible]

THR	VAL	ARG	SER	LYS	GLY	LYS
GLU	GLU	GLU	GLU	ALA	LEU	ALA
GLU	SER	LYS	GLU	GLY	GLN	VAL
TYR	LYS	LEU	ILE	LYS	ASP	THR
GLY	LEU	GLN	GLY	PRO	GLU	VAL
ASN	ALA	GLU	MET	LEU	LEU	ALA
MET	ASP	ARG	GLU	LEU	ASP	VAL
ILE	LEU	VAL	ARG	ILE	VAL	GLU
GLU	ARG	ALA	GLU	ILE	VAL	GLU
MET	GLY	LYS	GLY	ALA	GLY	LYS
ILE	ASN	ALA	THR	ASP	MET	ALA
LEU	GLU	GLY	LEU	VAL	GLN	LEU
PRO	ASP	GLY	GLU	GLU	PHE	SER
THR	GLN	VAL	ASP	GLY	ARG	PRO
ASN	ALA	ALA	LEU	ALA	GLY	CYS
VAL	VAL	ILE	GLN	LEU	TYR	SER
THR	ILE	LYS	ALA	ALA	LEU	ASP
ARG	ARG	LYS	LYS	THR	LEU	SER
SER	VAL	GLY	ARG	LEU	PRO	LYS
ALA	ALA	ALA	VAL	VAL	TYR	ALA
LEU	LEU	ALA	VAL	VAL	PHE	ILE
GLN	ARG	THR	ILE	ASN	ILE	ALA
TYR	ALA	GLU	ASN	THR	ASN	GLN
ALA	MET	VAL	LYS	MET	LYS	VAL
ALA	GLU	GLU	ASP	ARG	PRO	GLY
SER	ALA	MET	THR	GLY	GLU	THR
VAL	PRO	LYS	THR	ILE	THR	ILE
ALA	LEU	GLU	THR	VAL	GLY	SER
GLY	GLN	LYS	ILE	LYS	ALA	ALA
LEU	ARG	LYS	ILE	VAL	VAL	ASN
GLU	GLN	LYS	ILE	VAL	VAL	ASN
THR	ASN	GLU	GLY	VAL	GLU	ASP
CYS	CYS	ASP	GLU	ALA	PRO	VAL
GLU	GLY	ALA	GLU	PRO	PHE	GLY
MET	GLY	LEU	ALA	GLY	ILE	LYS
VAL	GLU	HIS	ALA	PHE	LEU	LEU
THR	PRO	ALA	ILE	GLY	LEU	ILE
ASP	SER	THR	GLN	ASP	ALA	ALA
PRO	VAL	ARG	GLY	ARG	ASP	GLU
	ALA	ALA	VAL	LYS	LYS	ALA
	ASN	VAL	ALA	ALA	ILE	ASP
	THR	GLU	GLN	MET	SER	LYS
	VAL	GLU	ILE	LEU	ASN	VAL
	LYS	GLY	ARG	GLN	ILE	GLY
	GLY	VAL	GLN	ILE	ARG	LYS
	ASP	ALA	ILE	ALA	MET	GLY
	ASN	GLY	GLU	THR	LEU	VAL
	TYR	GLY	ALA	LEU	PRO	ILE
	THR	VAL	THR	THR	VAL	THR
	TYR	ALA	SER	GLY	LEU	VAL
	ASN	LEU	ASP	THR	ALA	ASP
	ALA	ARG	TYR	VAL	VAL	GLY

- Molecule 1: 60 kDa chaperonin

Chain 2-M:  100%

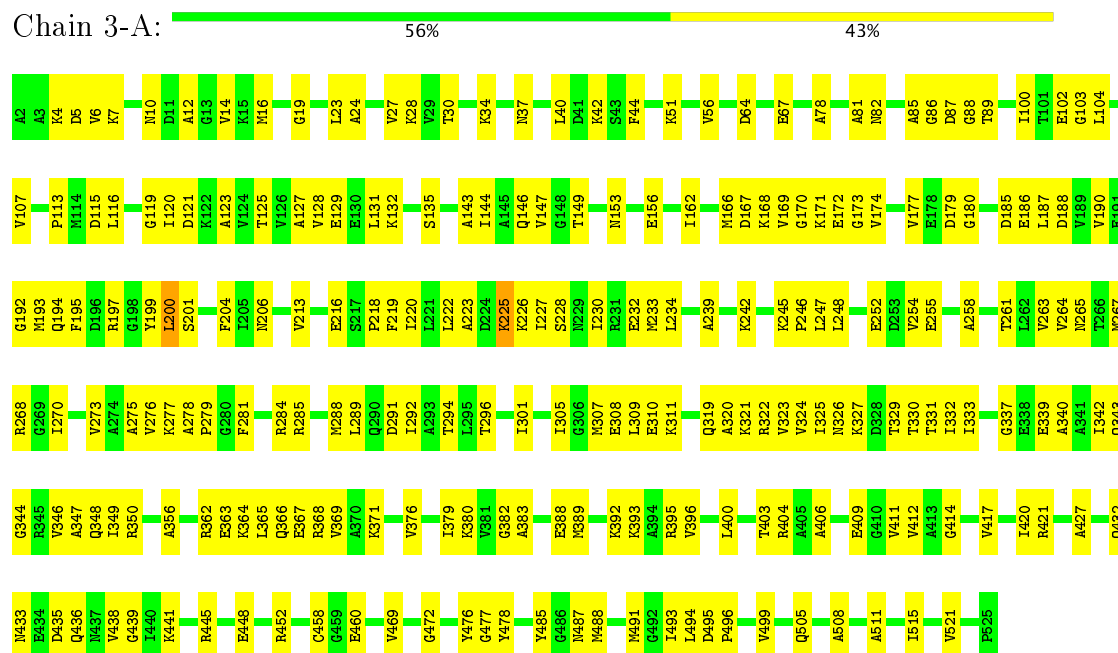
[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 2-N:  100%

THR	VAL	ARG	SER	LYS	GLY	LEU	ALA	ALA	LEU	ASP	LEU	ALA
GLU	ALA	GLU	GLU	ALA	LEU	GLN	GLY	GLY	GLN	GLU	GLY	ALA
GLU	SER	LYS	LYS	GLY	LYS	ASP	THR	VAL	VAL	GLU	ASP	ALA
TYR	LYS	GLN	ILE	LYS	PRO	GLY	LEU	THR	GLY	VAL	PHE	VAL
GLY	LEU	GLN	GLY	PRO	LEU	LEU	LEU	VAL	LEU	ALA	LYS	ASP
ASN	ALA	GLU	MET	LEU	MET	GLY	LEU	VAL	ASP	GLN	ASN	LYS
ASP	ASP	ARG	GLU	LEU	ASP	VAL	GLY	VAL	VAL	MET	GLY	PHE
MET	ASP	ARG	GLU	LEU	GLY	LEU	LEU	VAL	VAL	GLY	ASN	GLY
ILE	LEU	VAL	LEU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLY	GLY
ASP	ARG	LYS	GLU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLY	ASN
MET	GLY	ALA	GLU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLY	ASN
GLN	GLN	LEU	ALA	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA
ILE	ASN	ALA	THR	ASP	GLY	GLY	THR	VAL	MET	ALA	GLY	GLY
LEU	GLU	GLY	LEU	VAL	LEU	VAL	VAL	VAL	GLN	VAL	LEU	VAL
ASP	ASP	THR	GLU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	LYS	LYS
PRO	GLN	VAL	ASP	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	GLU	VAL	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
CYS	CYS	ALA	GLU	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
GLY	GLY	ALA	GLU	PRO	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
THR	THR	HIS	ALA	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
ASP	PRO	ALA	ILE	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
PRO	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
VAL	VAL	ARG	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
PRO	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	VAL	THR	GLY	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LEU	VAL	THR	GLY	ARG	ASP	ASP</						

- Molecule 1: 60 kDa chaperonin



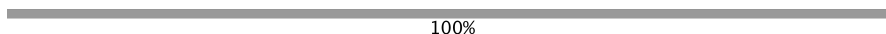
- Molecule 1: 60 kDa chaperonin



[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 3-C:

[illegible]

THR  
GLU  
GLU  
TYR  
GLY  
ASN  
MET  
ILE  
ASP  
MET  
GLY  
ILE  
LEU  
ASP  
PRO  
THR  
LYS  
VAL  
THR  
ARG  
SER  
ALA  
LEU  
GLN  
TYR  
ALA  
ALA  
SER  
VAL  
VAL  
ALA  
GLY  
LEU  
MET  
ILE  
THR  
THR  
GLU  
CYS  
MET  
VAL  
THR  
ASP  
LEU  
PRO

- Molecule 1: 60 kDa chaperonin

Chain 3-D:  100%

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 3-E:  100%

[illegible]

THR	GLU	GLU	TYR	GLY	ASN	MET	ILE	ASP	MET	GLY	ILE	LEU	ASP	PRO	THR	LYS	VAL	THR	ARG	SER	ALA	LEU	GLN	TYR	ALA	ALA	SER	VAL	ALA	GLY	LEU	MET	ILE	THR	THR	GLU	CYS	MET	VAL	THR	ASP	LEU	PRO
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- Molecule 1: 60 kDa chaperonin

Chain 3-F:  100%

THR	GLU	GLU	TYR	GLY	ASN	MET	MET	ASP	MET	GLY	ILE	LEU	ASP	PRO	THR	LYS	VAL	THR	ARG	SER	SER	ALA	LEU	GLN	TYR	ALA	ALA	SER	VAL	ALA	GLY	LEU	MET	ILE	THR	THR	GLU	CYS	MET	MET	VAL	THR	ASP	LEU	PRO
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- Molecule 1: 60 kDa chaperonin

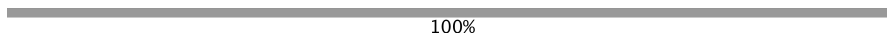
Chain 3-G:  100%

[illegible]

THR	VAL	ARG	SER	LYS
GLU	ALA	GLU	GLU	ALA
GLU	SER	LYS	GLU	GLY
TYR	LYS	LEU	ILE	LYS
GLY	LEU	GLN	GLY	PRO
ASN	ALA	GLU	MET	LEU
MET	ASP	ARG	GLU	LEU
ILE	LEU	VAL	LEU	ILE
ASP	ARG	ALA	GLU	ILE
MET	GLY	LYS	LYS	ALA
GLY	GLN	LEU	ALA	GLU
ILE	ASN	ALA	THR	ASP
LEU	GLU	GLY	LEU	VAL
ASP	ASP	GLY	GLU	GLY
PRO	GLN	VAL	ASP	GLY
THR	ASN	ALA	LEU	GLU
LYS	VAL	VAL	GLY	ALA
SER	VAL	GLY	ARG	THR
ALA	ALA	ALA	VAL	VAL
LEU	LEU	ALA	VAL	VAL
GLN	ARG	THR	ILE	ASN
TYR	ALA	GLU	ASN	THR
ALA	MET	VAL	LYS	MET
ALA	GLU	GLU	ASP	ARG
SER	ALA	MET	THR	GLY
VAL	PRO	LYS	THR	ILE
ALA	LEU	GLU	THR	VAL
GLY	ARG	LYS	ILE	LYS
LEU	GLN	LYS	ILE	VAL
MET	ILE	ALA	ASP	ALA
ILE	VAL	ARG	GLY	ALA
THR	LEU	VAL	VAL	VAL
THR	ASN	GLU	GLY	LYS
GLU	CYS	ASP	GLU	ALA
CYS	GLY	ALA	GLU	PRO
MET	GLU	LEU	ALA	GLY
VAL	GLU	HIS	ALA	PHE
THR	PRO	ALA	ILE	GLY
ASP	SER	THR	GLN	ASP
LEU	VAL	ARG	GLY	ARG
PRO	VAL	ALA	VAL	LYS
	ALA	ALA	ALA	LYS
	ASN	VAL	ALA	MET
	THR	GLU	GLN	LEU
	VAL	GLU	ILE	GLN
	LYS	GLY	ARG	ASP
	GLY	VAL	GLN	ILE
	GLY	ALA	ILE	ALA
	ASP	ALA	GLU	THR
	ASN	GLY	GLU	LEU
	TYR	GLY	ALA	THR
	GLY	VAL	THR	GLY
	THR	ALA	SER	GLY
	ASN	LEU	ASP	THR
	ALA	ILE	TYR	THR
	ALA	ARG	ASP	ILE

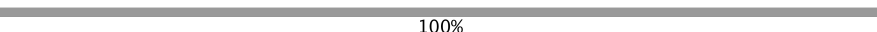
- Molecule 1: 60 kDa chaperonin

Chain 3-H:

[illegible]

- Molecule 1: 60 kDa chaperonin

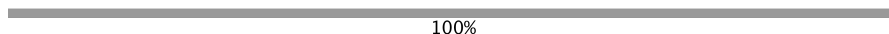
Chain 3-I:

[illegible]

THR	VAL	ARG	SER	LYS	GLY	LYS
GLU	GLU	GLU	GLU	ALA	LEU	ALA
GLU	SER	LYS	GLU	GLY	GLN	VAL
TYR	LYS	LEU	ILE	LYS	ASP	THR
GLY	LEU	GLN	GLY	PRO	GLU	ALA
ASN	ALA	GLU	MET	LEU	LEU	ALA
MET	ASP	ARG	GLU	LEU	ASP	VAL
ILE	LEU	VAL	LEU	ILE	VAL	GLU
GLU	ARG	ALA	GLU	ILE	VAL	GLU
MET	GLY	LYS	GLY	ALA	GLY	LYS
ILE	ASN	ALA	THR	ASP	MET	ALA
LEU	GLU	GLY	LEU	VAL	GLN	LEU
PRO	ASP	GLY	GLU	GLU	PHE	SER
THR	GLN	VAL	ASP	GLY	ARG	PRO
ASN	ALA	ALA	LEU	ALA	GLY	CYS
VAL	VAL	ILE	GLY	LEU	TYR	SER
THR	ILE	LYS	ALA	ALA	LEU	ASP
ARG	ARG	LYS	ALA	THR	LEU	GLN
TYR	THR	THR	ILE	ASN	ILE	ALA
GLN	ARG	THR	ILE	ASN	ASN	GLN
ALA	MET	VAL	LYS	MET	LYS	VAL
ALA	GLU	GLU	ASP	ARG	PRO	GLY
ALA	ALA	ALA	ASP	GLY	GLU	THR
SER	ALA	MET	THR	GLY	THR	ILE
VAL	PRO	LYS	THR	ILE	THR	ILE
ALA	LEU	GLU	THR	VAL	GLY	SER
GLY	GLY	LYS	ILE	LYS	ALA	ALA
LEU	ARG	LYS	ILE	VAL	VAL	ASN
THR	ILE	ALA	ILE	ALA	GLU	SER
THR	VAL	VAL	GLY	ALA	LEU	ASP
THR	ASN	GLU	GLY	VAL	GLU	THR
CYS	CYS	GLU	ASP	ALA	PRO	VAL
GLY	GLY	ALA	GLU	PRO	PHE	GLY
MET	GLU	LEU	ALA	GLY	ILE	LYS
VAL	GLU	HIS	ALA	PHE	LEU	LEU
THR	PRO	ALA	ILE	GLY	LEU	ILE
ASP	SER	THR	GIN	ASP	ALA	ALA
PRO	VAL	ARG	GLY	ARG	ASP	GLU
	ALA	ALA	VAL	LYS	LYS	ALA
	ALA	VAL	ALA	LYS	ASP	MET
	ASN	VAL	ALA	ALA	ILE	LYS
	THR	GLU	GLN	MET	SER	LYS
	VAL	GLU	ILE	LEU	ASN	VAL
	LYS	GLY	ARG	GLN	ILE	GLY
	GLY	VAL	GLN	ILE	ARG	LYS
	ASP	ALA	ILE	ALA	MET	GLY
	GLY	GLY	GLU	THR	LEU	VAL
	ASN	GLY	GLU	LEU	PRO	THR
	TYR	GLY	ALA	THR	VAL	VAL
	THR	VAL	THR	GLY	LEU	THR
	TYR	ALA	SER	GLY	GLU	VAL
	ASN	LEU	ASP	THR	ALA	ASP
	ALA	ILE	TYR	VAL	VAL	GLY
	ALA	ARG	ASN	ILE	VAL	THR

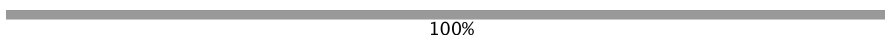
- Molecule 1: 60 kDa chaperonin

Chain 3-J:

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 3-K:

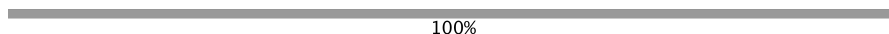




[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 3-L:

[illegible]

THR GLU GLU TYR GLY ASN MET ILE ASP MET GLY ILE LEU ASP PRO THR LYS VAL THR ARG SER ALA LEU GLN TYR ALA ALA VAL ALA GLY LEU MET ILE THR THR GLU CYS MET VAL THR ASP LEU PRO

- Molecule 1: 60 kDa chaperonin

Chain 3-M:  100%

ALA	ALA	ALA	LYS	ASP	VAL	LYS	PHE	GLY	GLY	ASN	ASP	ALA	GLY	VAL	VAL	LYS	NET	LEU	ARG	GLY	VAL	ASN	VAL	VAL	LEU	ALA	ASP	ALA	VAL	LYS	VAL	THR	THR	LEU	GLY	GLY	PRO	LYS	GLY	ARG	ASN	VAL	VAL	VAL	LEU	LEU	ASP	LYS	LYS	SER	PHE	GLY	GLY	ALA	ALA	PRO	THR	THR	THR	LYS	ASP	GLY	VAL	SER	VAL	ALA	ALA	ARG	GLU	ILE	ILE
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LEU	ASP	LYS	PHE	GLU	ASN	MET	GLY	ALA	ALA	GLN	MET	VAL	LYS	GLU	VAL	ALA	SER	LYS	ALA	ASN	ASP	ALA	ALA	GLY	GLY	THR	THR	THR	THR	ALA	VAL	LEU	ALA	GLN	ALA	ILE	ILE	THR	GLU	GLY	LEU	LYS	ALA	VAL	ALA	ALA	ALA	GLY	MET	ASN	PRO	MET	ASP	LEU	LYS	ARG	GLY	ILE
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LYS	ALA	VAL	THR	VAL	ALA	VAL	GLU	GLU	LEU	LYS	ALA	LEU	SER	VAL	PRO	ASP	SER	LYS	ALA	ILE	ALA	GLN	GLY	THR	ILE	SER	ASN	SER	ASP	GLU	THR	VAL	VAL	GLY	LYS	ILE	ALA	LYS	VAL	VAL	ASP	LYS	VAL	THR	VAL	GLU	ASP	GLY
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GLY LEU GLN GLN ASP ASP LEU LEU VAL VAL GLU GLU MET MET GLN PHE ASP ASP ARG ARG TYR LEU LEU SER SER TYR TYR PHE PHE ILE ILE ASN ASN LYS LYS PRO PRO GLU GLU THR THR GLY GLY ALA ALA VAL VAL GLU GLU LEU LEU SER SER PRO PRO PHE PHE ILE ILE ILE ILE SER SER ASN ASN ILE ILE LYS LYS ASP ASP ALA ALA LEU LEU LEU LEU LEU LEU VAL VAL GLU GLU ALA ALA VAL VAL

LYS	ALA	GLY	LYS	PRO	LEU	LEU	ILE	ILE	ALA	GLU	ASP	VAL	GLU	GLY	GLU	ALA	ALA	LEU	ALA	THR	LEU	VAL	VAL	ASN	THR	MET	ARG	GLY	ILE	VAL	LYS	VAL	ALA	ALA	ALA	VAL	LYS	ALA	PRO	GLY	GLY	PHE	GLY	GLY	ASP	ARG	ARG	LYS	ALA	ALA	MET	LEU	GLN	ASP	ILE	ALA	THR	LEU	THR	GLY	GLY	THR	VAL
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SER	GLU	GLU	ILE	GLY	MET	GLU	LEU	GLU	LYS	ALA	THR	LEU	ASP	VAL	VAL	ASN	LYS	ASP	THR	THR	ILE	ILE	ASP	GLY	VAL	GLY	GLU	GLU	ALA	ALA	ILE	GLN	GLY	ARG	VAL	VAL	GLN	GLN	ILE	GLN	ILE	ARG	GLN	GLN	ILE	GLU	GLU	ALA	THR	THR	SER	ASP	THR
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ARG GLU LYS LEU GLN GLU ARG VAL VAL LYS LYS ALA ALA GLY GLY VAL VAL ILE LYS VAL GLY GLY ALA ALA VAL VAL THR GLU GLU VAL GLU GLU MET LYS GLU LYS LYS ALA ALA ARG ARG VAL GLU ASP ALA ALA LEU HIS HIS ALA ALA THR ARG ALA ALA VAL VAL VAL GLU GLU GLY GLY VAL VAL VAL GLY GLY ALA ALA LEU ILE

VAL	ALA	SER	LYS	LEU	ALA	ASP	LEU	ARG	GLY	GLN	ASN	GLU	ASP	GLN	ASN	VAL	GLY	LYS	VAL	LEU	ARG	ALA	ALA	GLU	MET	GLY	ALA	PRO	LEU	ARG	GLN	ILE	VAL	LEU	ASN	CYS	GLY	GLU	GLU	GLU	PRO	SER	VAL	VAL	ALA	ALA	ASN	THR	VAL	LYS	GLY	GLY	ASP	GLY	ASN	TYR	GLY	TYR	ASN	ALA
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THR	GLU	GLU	TYR	GLY	ASN	MET	ILE	ASP	MET	GLY	ILE	LEU	ASP	PRO	THR	LYS	VAL	THR	ARG	SER	SER	ALA	LEU	GLN	TYR	ALA	ALA	SER	VAL	ALA	GLY	LEU	MET	ILE	THR	THR	GLU	CYS	MET	MET	VAL	THR	ASP	LEU	PRO
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- Molecule 1: 60 kDa chaperonin

Chain 3-N:  100%

[illegible]

LEU	GLU	ASP	LYS	PHS	GLU	ASN	MET	GLY	ALA	ALA	GLN	VAL	VAL	GLU	GLU	VAL	ALA	ALA	SER	LYS	ALA	ASN	ASP	ASP	ALA	ALA	GLY	GLY	THR	THR	THR	ALA	THR	VAL	LEU	ALA	GLN	ALA	ILE	ILE	THR	THR	GLU	GLY	LEU	LYS	ALA	VAL	VAL	ALA	ALA	ALA	GLY	MET	ASN	PRO	MET	ASP	LYS	ARG	GLY	ILE
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LYS	ALA	VAL	THR	VAL	ALA	VAL	GLU	GLU	LEU	LYS	ALA	LEU	SER	VAL	PRO	CYS	SER	ASP	SER	LYS	ALA	ILE	ALA	GLN	GLY	THR	ILE	SER	ASN	SER	ASP	GLU	THR	VAL	GLY	LYS	ILE	ALA	GLU	ALA	MET	ASP	LYS	VAL	GLY	LYS	GLU	GLY	VAL	ILE	THR	VAL	GLU	ASP	GLY
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GLY	LEU	GLN	ASP	GLU	LEU	ASP	VAL	GLU	GLY	GLY	MET	GLN	PHE	ASP	ARG	GLY	TYR	LEU	SER	PRO	PRO	THR	GLU	GLY	ALA	VAL	GLU	LEU	GLU	SER	PRO	PRO	PHE	ILE	ILE	SER	ASN	ILE	ILE	ARG	GLU	GLU	MET	LEU	PRO	VAL	LEU	GLU	ALA	VAL
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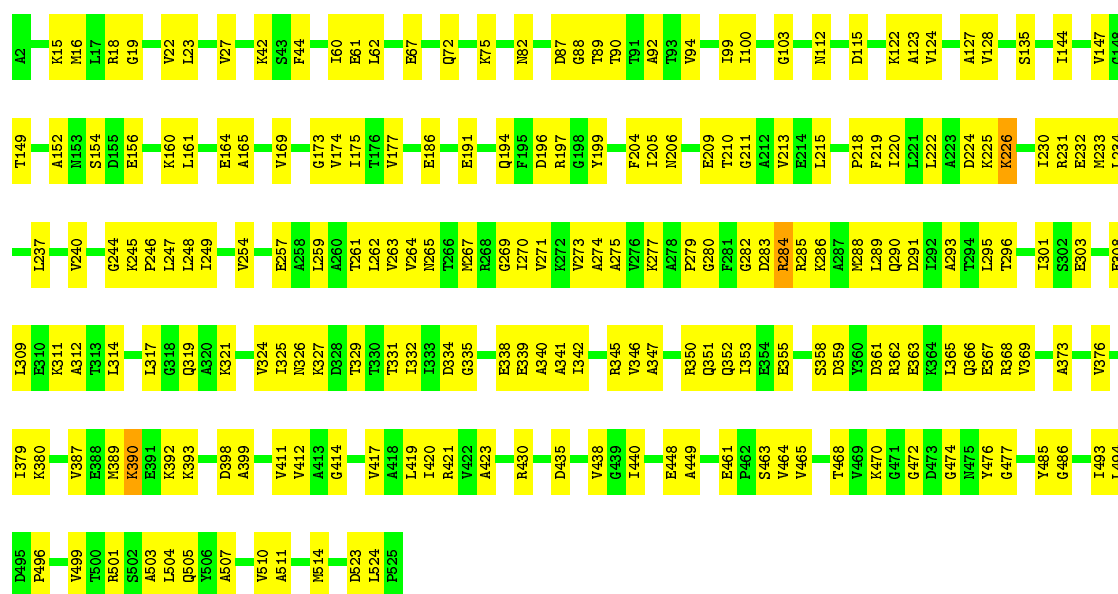
LYS ALA LYS GLY LYS PRO PRO LEU LEU ILE ILE ALA ALA GLU GLU ASP VAL VAL GLU GLY GLY GLU GLU ALA ALA ASN THR THR MET MET ARG ARG GLY GLY PHE PHE GLY GLY ASP ASP ARG ARG ARG LYS LYS ALA ALA MET MET LEU LEU GLN GLN ASP ASP ILE ILE ALA ALA THR THR LEU LEU THR GLY GLY GLY GLY THR THR VAL VAL

[illegible]

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-A:  61% 39%



- Molecule 1: 60 kDa chaperonin

Chain 4-B:  100%

[illegible]

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-C:  100%

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-D:  100%

[illegible]

THR	VAL	ARG	SER	LYS
GLU	ALA	GLU	GLU	ALA
GLU	SER	LYS	GLU	GLY
TYR	LYS	LEU	ILE	LYS
GLY	LEU	GLN	GLY	PRO
ASN	ALA	GLU	MET	LEU
MET	ASP	ARG	GLU	LEU
ILE	LEU	VAL	LEU	ILE
ASP	ARG	ALA	GLU	ILE
MET	GLY	LYS	LYS	ALA
GLY	GLN	LEU	ALA	GLU
ILE	ASN	ALA	THR	ASP
LEU	GLU	GLY	LEU	VAL
ASP	ASP	GLY	GLU	GLY
PRO	GLN	VAL	ASP	GLY
THR	ASN	ALA	LEU	GLU
LYS	VAL	VAL	GLY	ALA
SER	VAL	GLY	ARG	THR
ALA	ALA	ALA	VAL	VAL
LEU	LEU	ALA	VAL	VAL
GLN	ARG	THR	ILE	ASN
TYR	ALA	GLU	ASN	THR
ALA	MET	VAL	LYS	MET
ALA	GLU	GLU	ASP	ARG
SER	ALA	MET	THR	GLY
VAL	PRO	LYS	THR	ILE
ALA	LEU	GLU	THR	VAL
GLY	ARG	LYS	ILE	LYS
LEU	GLN	LYS	ILE	VAL
MET	ILE	ALA	ASP	ALA
ILE	VAL	ARG	GLY	ALA
THR	LEU	VAL	VAL	VAL
THR	ASN	GLU	GLY	LYS
GLU	CYS	ASP	GLU	ALA
CYS	GLY	ALA	GLU	PRO
MET	GLU	LEU	ALA	GLY
VAL	GLU	HIS	ALA	PHE
THR	PRO	ALA	ILE	GLY
ASP	SER	THR	GLN	ASP
LEU	VAL	ARG	GLY	ARG
PRO	VAL	ALA	ARG	LYS
	ALA	ALA	VAL	LYS
	ASN	VAL	ALA	MET
	THR	GLU	GLN	LEU
	VAL	GLU	ILE	GLN
	LYS	GLY	ARG	ASP
	GLY	VAL	GLN	ILE
	GLY	ALA	ILE	ALA
	ASP	ALA	GLU	THR
	ASN	GLY	GLU	LEU
	TYR	GLY	ALA	THR
	GLY	VAL	THR	GLY
	TYR	ALA	SER	GLY
	ASN	LEU	ASP	THR
	ALA	ILE	TYR	THR
	ALA	ARG	ASP	ILE

- Molecule 1: 60 kDa chaperonin

Chain 4-E:  100%

[illegible]

- Molecule 1: 60 kDa chaperonin

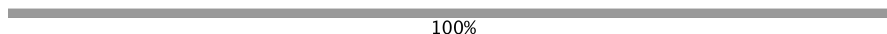
Chain 4-F:  100%

[illegible]

THR	VAL	ARG	SER	LYS	GLY	LYS
GLU	GLU	GLU	GLU	ALA	LEU	ALA
GLU	SER	LYS	GLU	GLY	GLN	VAL
TYR	LYS	LEU	ILE	LYS	ASP	THR
GLY	LEU	GLN	GLY	PRO	GLU	ALA
ASN	ALA	GLU	MET	LEU	LEU	ALA
MET	ASP	ARG	GLU	LEU	ASP	VAL
ILE	LEU	VAL	LEU	ILE	VAL	GLU
GLU	ARG	ALA	GLU	ILE	VAL	GLU
MET	GLY	LYS	GLY	ALA	GLY	LYS
ILE	ASN	ALA	THR	ASP	MET	ALA
LEU	GLU	GLY	LEU	VAL	GLN	LEU
PRO	ASP	GLY	GLU	GLU	PHE	SER
THR	GLN	VAL	ASP	GLY	ARG	PRO
ASN	ALA	ALA	LEU	ALA	GLY	CYS
VAL	VAL	ILE	GLN	LEU	TYR	SER
THR	ILE	LYS	ALA	ALA	LEU	ASP
ARG	ARG	LYS	ALA	THR	LEU	SER
TYR	THR	THR	ILE	ASN	ILE	ALA
GLN	ARG	THR	ILE	ASN	ASN	GLN
ALA	MET	VAL	LYS	MET	LYS	VAL
ALA	GLU	GLU	ASP	ARG	PRO	GLY
ALA	ALA	ALA	VAL	VAL	TYR	ALA
SER	ALA	MET	THR	VAL	GLY	THR
VAL	PRO	LYS	THR	ILE	THR	ILE
ALA	LEU	GLU	THR	VAL	GLY	SER
GLY	GLY	LYS	ILE	LYS	ALA	ALA
LEU	ARG	LYS	ILE	VAL	VAL	ASN
THR	ILE	ALA	ASP	ALA	GLU	SER
THR	LEU	VAL	GLY	VAL	GLU	ASP
THR	ASN	GLU	GLY	LYS	SER	THR
CYS	CYS	ASP	GLU	ALA	PRO	VAL
GLY	GLY	ALA	GLU	PRO	PHE	GLY
MET	GLU	LEU	ALA	GLY	ILE	LYS
VAL	GLU	HIS	ALA	PHE	LEU	LEU
THR	PRO	ALA	ILE	GLY	LEU	ILE
ASP	SER	THR	GLN	ASP	ALA	ALA
PRO	VAL	ARG	GLY	ARG	ASP	GLU
	ALA	ALA	VAL	LYS	LYS	ALA
	ASN	VAL	ALA	ALA	ILE	ASP
	THR	GLU	GLN	MET	SER	LYS
	VAL	GLU	ILE	LEU	ASN	VAL
	LYS	GLY	ARG	GLN	ILE	GLY
	GLY	VAL	GLN	ILE	ARG	LYS
	ASP	ALA	ILE	ALA	MET	GLY
	ASN	GLY	GLU	THR	LEU	VAL
	TYR	GLY	ALA	LEU	PRO	ILE
	THR	VAL	THR	THR	VAL	THR
	TYR	ALA	SER	GLY	GLU	VAL
	ASN	LEU	ASP	THR	ALA	ASP
	ALA	ARG	TYR	VAL	VAL	GLY
	ALA	ARG	ASN	ILE	ALA	THR

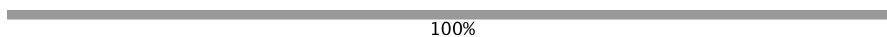
- Molecule 1: 60 kDa chaperonin

Chain 4-G:

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-H:



[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-I:

100%

[illegible]





THR	VAL	ARG
GLU	ALA	GLU
GLU	SER	LYS
TYR	LYS	LEU
GLY	LEU	GLN
ASN	ALA	GLU
MET	ASP	ARG
ILE	LEU	VAL
ASP	ARG	ALA
MET	GLY	LYS
GLY	GLN	LEU
ILE	ASN	ALA
LEU	GLU	GLY
ASP	ASP	GLY
PRO	GLN	VAL
THR	ASN	ALA
LYS	VAL	VAL
VAL	GLY	ILE
THR	ILE	LYS
ARG	LYS	VAL
SER	VAL	GLY
ALA	ALA	ALA
ALA	LEU	ALA
GLN	ARG	THR
TYR	ALA	GLU
ALA	MET	VAL
ALA	GLU	GLU
SER	ALA	MET
VAL	PRO	LYS
ALA	LEU	GLU
GLY	ARG	LYS
LEU	ILE	ALA
ILE	VAL	ARG
THR	LEU	VAL
THR	ASN	GLU
GLU	CYS	ASP
CYS	GLY	ALA
MET	GLU	LEU
VAL	GLU	HIS
THR	PRO	ALA
ASP	SER	THR
LEU	VAL	ARG
PRO	VAL	ALA
	ASN	VAL
	THR	GLU
	VAL	GLY
	LYS	VAL
	GLY	VAL
	ASP	ALA
	GLY	GLY
	ASN	GLY
	TYR	GLY
	GLY	VAL
	ASN	LEU
	THR	ALA
	VAL	ILE
	ALA	ARG

- Molecule 1: 60 kDa chaperonin

Chain 4-L:  100%

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-M:  100%

[illegible]

THR	VAL	ARG	SER	LYS
GLU	ALA	GLU	GLU	ALA
GLU	SER	LYS	GLU	GLY
TYR	LYS	LEU	ILE	LYS
GLY	LEU	GLN	GLY	PRO
ASN	ALA	GLU	MET	LEU
MET	ASP	ARG	GLU	LEU
ILE	LEU	VAL	LEU	ILE
ASP	ARG	VAL	LEU	ILE
MET	GLY	LYS	LYS	ALA
GLY	GLN	LEU	ALA	GLU
ILE	ASN	LEU	THR	ASP
LEU	GLU	GLY	LEU	VAL
ASP	ASP	GLY	GLU	GLY
PRO	GLN	VAL	ASP	GLY
THR	ASN	ALA	LEU	GLU
LYS	VAL	VAL	GLY	ALA
VAL	GLY	ILE	GLN	LEU
THR	ILE	LYS	ALA	ALA
ARG	LYS	VAL	LYS	THR
SER	VAL	GLY	ARG	LEU
ALA	ALA	ALA	VAL	VAL
LEU	LEU	ALA	VAL	VAL
GLN	ARG	THR	ILE	ASN
TYR	ALA	GLU	ASN	THR
ALA	MET	VAL	LYS	MET
ALA	ALA	GLU	ASP	ARG
SER	SER	ALA	MET	GLY
VAL	PRO	LYS	THR	ILE
ALA	LEU	GLU	THR	VAL
GLY	ARG	LYS	ILE	LYS
ILE	GLN	LYS	ILE	VAL
ILE	ILE	ALA	ASP	ALA
THR	VAL	ARG	GLY	ALA
THR	LEU	VAL	VAL	VAL
THR	ASN	GLU	GLY	LYS
GLU	CYS	ASP	GLU	ALA
THR	GLY	ALA	GLU	ALA
CYS	GLY	LEU	ALA	PRO
MET	MET	LEU	ALA	GLY
VAL	GLU	HIS	ALA	GLY
THR	PRO	ALA	ILE	PHE
THR	THR	THR	ALA	GLY
ASP	SER	THR	GLN	ASP
LEU	VAL	ARG	GLY	ARG
PRO	VAL	ALA	ARG	ARG
	ALA	ALA	VAL	LYS
	ASN	VAL	ALA	LYS
	THR	GLU	GLN	MET
	VAL	GLY	ILE	LEU
	LYS	GLY	ARG	GLN
	GLY	VAL	GLN	ASP
	ASP	ALA	ILE	ALA
	ASN	GLY	GLU	THR
	TYR	GLY	GLU	LEU
	THR	GLY	ALA	THR
	TYR	VAL	THR	GLY
	TYR	ALA	SER	GLY
	ASN	LEU	ASP	THR
	ALA	ILE	TYR	THR
	ALA	ARG	ASP	ILE

- Molecule 1: 60 kDa chaperonin

Chain 4-N:  100%

[illegible]

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	37367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	1-A	0.39	0/3879	0.57	0/5237
1	1-B	0.39	0/3879	0.57	0/5237
1	1-C	0.39	0/3879	0.57	0/5237
1	1-D	0.39	0/3879	0.57	0/5237
1	1-E	0.39	0/3879	0.57	0/5237
1	1-F	0.39	0/3879	0.57	0/5237
1	1-G	0.39	0/3879	0.57	0/5237
1	1-H	0.39	0/3879	0.57	0/5237
1	1-I	0.39	0/3879	0.57	0/5237
1	1-J	0.39	0/3879	0.57	0/5237
1	1-K	0.39	0/3879	0.57	0/5237
1	1-L	0.39	0/3879	0.57	0/5237
1	1-M	0.39	0/3879	0.57	0/5237
1	1-N	0.39	0/3879	0.57	0/5237
1	2-A	0.53	0/3879	0.67	1/5237 (0.0%)
1	3-A	0.45	0/3879	0.59	1/5237 (0.0%)
1	4-A	0.39	0/3879	0.54	0/5237
All	All	0.40	0/65943	0.58	2/89029 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	1-B	0	1
1	1-C	0	1
1	1-D	0	1
1	1-E	0	1
1	1-F	0	1
1	1-G	0	1
1	1-H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-I	0	1
1	1-J	0	1
1	1-K	0	1
1	1-L	0	1
1	1-M	0	1
1	1-N	0	1
All	All	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	200	LEU	C-N-CA	-6.91	104.44	121.70
1	2-A	234	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	32	GLY	Peptide
1	1-B	32	GLY	Peptide
1	1-C	32	GLY	Peptide
1	1-D	32	GLY	Peptide
1	1-E	32	GLY	Peptide
1	1-F	32	GLY	Peptide
1	1-G	32	GLY	Peptide
1	1-H	32	GLY	Peptide
1	1-I	32	GLY	Peptide
1	1-J	32	GLY	Peptide
1	1-K	32	GLY	Peptide
1	1-L	32	GLY	Peptide
1	1-M	32	GLY	Peptide
1	1-N	32	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3851	0	3970	58	0
1	1-B	3851	0	3970	56	0
1	1-C	3851	0	3970	58	0
1	1-D	3851	0	3970	56	0
1	1-E	3851	0	3970	56	0
1	1-F	3851	0	3970	55	0
1	1-G	3851	0	3970	58	0
1	1-H	3851	0	3970	58	0
1	1-I	3851	0	3970	57	0
1	1-J	3851	0	3970	55	0
1	1-K	3851	0	3970	59	0
1	1-L	3851	0	3970	56	0
1	1-M	3851	0	3970	55	0
1	1-N	3851	0	3970	57	0
1	2-A	3851	0	3970	234	0
1	3-A	3851	0	3970	192	0
1	4-A	3851	0	3970	148	0
2	1-A	19	0	0	1	0
2	1-B	12	0	0	0	0
2	1-C	14	0	0	0	0
2	1-D	14	0	0	0	0
2	1-E	10	0	0	0	0
2	1-F	6	0	0	0	0
2	1-G	13	0	0	0	0
2	1-H	1	0	0	0	0
2	1-I	3	0	0	0	0
2	1-J	5	0	0	0	0
2	1-K	1	0	0	0	0
2	1-L	2	0	0	0	0
2	1-M	5	0	0	0	0
2	1-N	2	0	0	0	0
All	All	65574	0	67490	1323	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1323) 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:A:176:THR:O	1:A:377:ALA:HB3	1.56	1.04
1:A:221:LEU:O	1:A:248:LEU:CB	2.14	0.95
1:A:264:VAL:HA	1:A:267:MET:HG2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HE	1:A:279:PRO:HA	1.35	0.92
1:A:237:LEU:O	1:A:241:ALA:HB2	1.70	0.91
1:F:187:LEU:HA	1:F:378:VAL:O	1.72	0.90
1:N:187:LEU:HA	1:N:378:VAL:O	1.72	0.90
1:M:187:LEU:HA	1:M:378:VAL:O	1.72	0.90
1:E:187:LEU:HA	1:E:378:VAL:O	1.72	0.90
1:G:187:LEU:HA	1:G:378:VAL:O	1.72	0.90
1:H:187:LEU:HA	1:H:378:VAL:O	1.72	0.90
1:A:220:ILE:HB	1:A:318:GLY:O	1.72	0.90
1:I:187:LEU:HA	1:I:378:VAL:O	1.72	0.89
1:A:187:LEU:HA	1:A:378:VAL:O	1.72	0.89
1:D:187:LEU:HA	1:D:378:VAL:O	1.72	0.89
1:J:187:LEU:HA	1:J:378:VAL:O	1.72	0.89
1:A:282:GLY:H	1:A:285:ARG:HH21	1.19	0.89
1:B:187:LEU:HA	1:B:378:VAL:O	1.72	0.89
1:L:187:LEU:HA	1:L:378:VAL:O	1.72	0.89
1:C:187:LEU:HA	1:C:378:VAL:O	1.72	0.88
1:K:187:LEU:HA	1:K:378:VAL:O	1.72	0.88
1:A:220:ILE:HG22	1:A:248:LEU:HB3	1.56	0.88
1:L:185:ASP:HA	1:L:380:LYS:O	1.78	0.83
1:D:185:ASP:HA	1:D:380:LYS:O	1.78	0.83
1:E:185:ASP:HA	1:E:380:LYS:O	1.78	0.83
1:A:427:ALA:O	1:A:441:LYS:NZ	2.11	0.83
1:M:185:ASP:HA	1:M:380:LYS:O	1.78	0.83
1:G:185:ASP:HA	1:G:380:LYS:O	1.78	0.83
1:H:185:ASP:HA	1:H:380:LYS:O	1.78	0.83
1:F:185:ASP:HA	1:F:380:LYS:O	1.78	0.83
1:A:185:ASP:HA	1:A:380:LYS:O	1.78	0.82
1:K:185:ASP:HA	1:K:380:LYS:O	1.78	0.82
1:N:185:ASP:HA	1:N:380:LYS:O	1.78	0.82
1:C:185:ASP:HA	1:C:380:LYS:O	1.78	0.82
1:I:185:ASP:HA	1:I:380:LYS:O	1.78	0.82
1:J:185:ASP:HA	1:J:380:LYS:O	1.78	0.82
1:B:185:ASP:HA	1:B:380:LYS:O	1.78	0.82
1:A:377:ALA:HB1	1:A:379:ILE:HG13	1.62	0.81
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.60	0.81
1:A:284:ARG:NH1	1:A:288:MET:SD	2.53	0.81
1:A:128:VAL:HG21	1:A:505:GLN:HE21	1.46	0.81
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.61	0.80
1:A:325:ILE:HG22	1:A:330:THR:HG23	1.63	0.80
1:A:186:GLU:HB2	1:A:380:LYS:HG3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:O	1:A:106:ALA:N	2.13	0.80
1:A:221:LEU:O	1:A:248:LEU:HB3	1.81	0.79
1:A:263:VAL:O	1:A:267:MET:N	2.16	0.79
1:A:249:ILE:HB	1:A:275:ALA:HA	1.65	0.79
1:A:285:ARG:O	1:A:288:MET:N	2.15	0.79
1:A:172:GLU:HA	1:A:404:ARG:HH12	1.48	0.78
1:A:421:ARG:NH1	1:A:469:VAL:O	2.17	0.77
1:A:214:GLU:OE2	1:A:322:ARG:NH2	2.17	0.77
1:A:448:GLU:OE2	1:A:470:LYS:NZ	2.16	0.77
1:A:220:ILE:HD11	1:A:296:THR:HG21	1.66	0.76
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.68	0.76
1:A:221:LEU:HD13	1:A:247:LEU:HD11	1.66	0.75
1:A:225:LYS:NZ	1:A:301:ILE:O	2.20	0.75
1:A:81:ALA:O	1:A:85:ALA:HB3	1.87	0.74
1:I:81:ALA:O	1:I:85:ALA:HB3	1.87	0.74
1:G:81:ALA:O	1:G:85:ALA:HB3	1.87	0.74
1:H:81:ALA:O	1:H:85:ALA:HB3	1.87	0.74
1:L:81:ALA:O	1:L:85:ALA:HB3	1.87	0.74
1:D:81:ALA:O	1:D:85:ALA:HB3	1.87	0.74
1:M:81:ALA:O	1:M:85:ALA:HB3	1.87	0.74
1:B:81:ALA:O	1:B:85:ALA:HB3	1.87	0.73
1:E:81:ALA:O	1:E:85:ALA:HB3	1.87	0.73
1:J:81:ALA:O	1:J:85:ALA:HB3	1.87	0.73
1:A:30:THR:OG1	1:A:51:LYS:O	2.06	0.73
1:F:81:ALA:O	1:F:85:ALA:HB3	1.87	0.73
1:N:81:ALA:O	1:N:85:ALA:HB3	1.87	0.73
1:K:81:ALA:O	1:K:85:ALA:HB3	1.87	0.73
1:C:81:ALA:O	1:C:85:ALA:HB3	1.87	0.72
1:A:215:LEU:HD23	1:A:246:PRO:HB2	1.70	0.72
1:A:226:LYS:HG2	1:A:253:ASP:HB3	1.70	0.72
1:A:291:ASP:OD1	1:A:345:ARG:NH2	2.23	0.72
1:A:356:ALA:O	1:A:362:ARG:NH2	2.23	0.72
1:A:82:ASN:O	1:A:86:GLY:N	2.22	0.71
1:A:281:PHE:HA	1:A:285:ARG:HH21	1.54	0.71
1:A:112:ASN:HB3	1:A:115:ASP:HB2	1.71	0.71
1:A:321:LYS:HG2	1:A:334:ASP:HB2	1.73	0.71
1:A:308:GLU:OE1	1:A:310:GLU:N	2.23	0.71
1:A:291:ASP:OD1	1:A:345:ARG:NH1	2.24	0.71
1:A:194:GLN:O	1:A:371:LYS:NZ	2.21	0.71
1:A:362:ARG:O	1:A:366:GLN:N	2.23	0.71
1:A:349:ILE:HD11	1:A:365:LEU:HD22	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:O	1:A:248:LEU:HB2	1.90	0.70
1:A:85:ALA:HB1	1:A:499:VAL:HG22	1.72	0.70
1:A:261:THR:HA	1:A:264:VAL:HG12	1.73	0.70
1:A:189:VAL:HG13	1:A:375:GLY:HA3	1.74	0.70
1:A:322:ARG:O	1:A:333:ILE:HB	1.92	0.70
1:A:448:GLU:OE2	1:A:452:ARG:NH1	2.17	0.69
1:A:153:ASN:OD1	1:A:395:ARG:NH1	2.25	0.69
1:A:339:GLU:O	1:A:343:GLN:HB2	1.92	0.69
1:A:383:ALA:HB3	1:A:389:MET:HG3	1.72	0.69
1:A:9:GLY:O	1:A:13:GLY:N	2.22	0.69
1:A:152:ALA:HB2	1:A:399:ALA:HB2	1.75	0.69
1:A:369:VAL:O	1:A:373:ALA:N	2.25	0.69
1:A:128:VAL:HG23	1:A:501:ARG:HG3	1.74	0.69
1:A:432:GLN:N	1:A:436:GLN:OE1	2.20	0.68
1:A:219:PHE:HB2	1:A:245:LYS:HE2	1.75	0.68
1:A:221:LEU:HA	1:A:317:LEU:HD22	1.73	0.68
1:A:411:VAL:HG21	1:A:494:LEU:HD13	1.76	0.68
1:A:232:GLU:HG3	1:A:309:LEU:HB2	1.75	0.68
1:A:232:GLU:HB3	1:A:309:LEU:HD12	1.76	0.68
1:A:460:GLU:OE1	1:A:460:GLU:N	2.27	0.67
1:A:100:ILE:HD11	1:A:511:ALA:HA	1.74	0.67
1:A:179:ASP:O	1:A:380:LYS:HD2	1.94	0.67
1:B:176:THR:O	1:B:377:ALA:HB3	1.95	0.67
1:J:176:THR:O	1:J:377:ALA:HB3	1.95	0.67
1:A:219:PHE:H	1:A:245:LYS:HD3	1.60	0.67
1:A:192:GLY:HA3	1:A:376:VAL:HG23	1.76	0.67
1:A:176:THR:O	1:A:377:ALA:HB3	1.95	0.66
1:K:176:THR:O	1:K:377:ALA:HB3	1.95	0.66
1:A:323:VAL:HG12	1:A:332:ILE:HA	1.76	0.66
1:C:176:THR:O	1:C:377:ALA:HB3	1.95	0.66
1:F:176:THR:O	1:F:377:ALA:HB3	1.95	0.66
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.76	0.66
1:I:176:THR:O	1:I:377:ALA:HB3	1.95	0.66
1:A:378:VAL:HG22	1:A:380:LYS:HD3	1.76	0.66
1:L:176:THR:O	1:L:377:ALA:HB3	1.95	0.66
1:N:176:THR:O	1:N:377:ALA:HB3	1.95	0.66
1:D:176:THR:O	1:D:377:ALA:HB3	1.95	0.66
1:G:176:THR:O	1:G:377:ALA:HB3	1.95	0.66
1:E:176:THR:O	1:E:377:ALA:HB3	1.95	0.66
1:M:176:THR:O	1:M:377:ALA:HB3	1.95	0.66
1:H:176:THR:O	1:H:377:ALA:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:ND2	1:A:232:GLU:OE1	2.30	0.65
1:A:220:ILE:HD11	1:A:296:THR:HG21	1.78	0.65
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.79	0.64
1:A:262:LEU:HD22	1:A:273:VAL:HG11	1.79	0.64
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.79	0.64
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.79	0.64
1:J:247:LEU:HB3	1:J:273:VAL:HG22	1.79	0.64
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.79	0.64
1:H:247:LEU:HB3	1:H:273:VAL:HG22	1.79	0.64
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.79	0.64
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.79	0.64
1:N:247:LEU:HB3	1:N:273:VAL:HG22	1.79	0.64
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.79	0.64
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.79	0.64
1:A:230:ILE:HA	1:A:233:MET:HB3	1.80	0.64
1:K:247:LEU:HB3	1:K:273:VAL:HG22	1.79	0.64
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.79	0.64
1:A:365:LEU:O	1:A:369:VAL:N	2.26	0.64
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.79	0.64
1:A:66:PHE:HD1	1:A:520:MET:HE1	1.63	0.64
1:A:247:LEU:O	1:A:273:VAL:HA	1.98	0.64
1:A:87:ASP:OD1	1:A:88:GLY:N	2.28	0.63
1:A:119:GLY:HA3	1:A:439:GLY:HA3	1.80	0.63
1:A:280:GLY:HA3	1:A:284:ARG:HH12	1.62	0.63
1:A:479:ASN:OD1	1:A:480:ALA:N	2.31	0.63
1:A:166:MET:HE2	1:A:171:LYS:HA	1.81	0.63
1:A:228:SER:HA	1:A:258:ALA:HB2	1.81	0.63
1:A:232:GLU:OE2	1:A:310:GLU:N	2.32	0.63
1:A:61:GLU:OE1	1:A:72:GLN:NE2	2.32	0.62
1:A:197:ARG:HD2	1:A:277:LYS:HB3	1.81	0.62
1:A:76:GLU:O	1:A:79:SER:OG	2.11	0.62
1:D:152:ALA:HB2	1:D:399:ALA:HB2	1.82	0.62
1:L:152:ALA:HB2	1:L:399:ALA:HB2	1.82	0.62
1:A:339:GLU:HA	1:A:342:ILE:HG22	1.81	0.62
1:A:186:GLU:HB3	1:A:380:LYS:HB2	1.82	0.62
1:A:152:ALA:HB2	1:A:399:ALA:HB2	1.82	0.62
1:C:152:ALA:HB2	1:C:399:ALA:HB2	1.82	0.62
1:K:152:ALA:HB2	1:K:399:ALA:HB2	1.82	0.62
1:A:389:MET:O	1:A:393:LYS:N	2.27	0.62
1:B:152:ALA:HB2	1:B:399:ALA:HB2	1.82	0.62
1:E:152:ALA:HB2	1:E:399:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:HB2	1:G:399:ALA:HB2	1.82	0.62
1:I:152:ALA:HB2	1:I:399:ALA:HB2	1.82	0.62
1:M:152:ALA:HB2	1:M:399:ALA:HB2	1.82	0.62
1:A:321:LYS:HB3	1:A:334:ASP:HB2	1.81	0.62
1:F:152:ALA:HB2	1:F:399:ALA:HB2	1.82	0.62
1:H:152:ALA:HB2	1:H:399:ALA:HB2	1.82	0.62
1:J:152:ALA:HB2	1:J:399:ALA:HB2	1.82	0.62
1:A:237:LEU:O	1:A:241:ALA:CB	2.46	0.62
1:N:152:ALA:HB2	1:N:399:ALA:HB2	1.82	0.61
1:A:124:VAL:HG22	1:A:504:LEU:HD21	1.80	0.61
1:A:186:GLU:HB2	1:A:380:LYS:CG	2.28	0.61
1:A:104:LEU:HA	1:A:107:VAL:HG12	1.80	0.61
1:A:116:LEU:O	1:A:120:ILE:N	2.25	0.61
1:A:100:ILE:O	1:A:103:GLY:N	2.34	0.61
1:A:177:VAL:HG22	1:A:379:ILE:HD12	1.81	0.61
1:A:82:ASN:OD1	1:A:89:THR:OG1	2.18	0.61
1:A:326:ASN:OD1	1:A:327:LYS:N	2.34	0.61
1:A:376:VAL:HG12	1:A:377:ALA:H	1.66	0.61
1:A:417:VAL:O	1:A:420:ILE:HG22	2.01	0.60
1:A:37:ASN:OD1	1:A:51:LYS:NZ	2.29	0.60
1:A:219:PHE:HB2	1:A:245:LYS:CE	2.31	0.60
1:A:230:ILE:HG23	1:A:257:GLU:HG3	1.82	0.60
1:A:178:GLU:HB2	1:A:378:VAL:HG23	1.83	0.60
1:K:232:GLU:HB3	1:K:309:LEU:HB2	1.84	0.60
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.84	0.60
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.84	0.60
1:A:199:TYR:HB3	1:A:325:ILE:HD13	1.83	0.60
1:A:478:TYR:HB2	1:A:485:TYR:HE1	1.66	0.60
1:A:5:ASP:OD1	1:A:6:VAL:N	2.33	0.60
1:C:232:GLU:HB3	1:C:309:LEU:HB2	1.84	0.60
1:N:232:GLU:HB3	1:N:309:LEU:HB2	1.84	0.60
1:E:232:GLU:HB3	1:E:309:LEU:HB2	1.84	0.60
1:F:232:GLU:HB3	1:F:309:LEU:HB2	1.84	0.60
1:L:232:GLU:HB3	1:L:309:LEU:HB2	1.84	0.60
1:D:232:GLU:HB3	1:D:309:LEU:HB2	1.84	0.60
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.84	0.60
1:M:232:GLU:HB3	1:M:309:LEU:HB2	1.84	0.60
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.84	0.60
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.84	0.60
1:B:232:GLU:HB3	1:B:309:LEU:HB2	1.84	0.60
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HA	1:A:307:MET:HE3	1.83	0.60
1:A:347:ALA:HA	1:A:350:ARG:HB2	1.83	0.60
1:J:232:GLU:HB3	1:J:309:LEU:HB2	1.84	0.60
1:A:143:ALA:HA	1:A:146:GLN:HG2	1.84	0.60
1:A:145:ALA:HB2	1:A:163:ALA:HB2	1.84	0.59
1:G:232:GLU:HB3	1:G:309:LEU:HB2	1.84	0.59
1:H:177:VAL:HG22	1:H:379:ILE:HD12	1.83	0.59
1:H:232:GLU:HB3	1:H:309:LEU:HB2	1.84	0.59
1:K:177:VAL:HG22	1:K:379:ILE:HD12	1.83	0.59
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.84	0.59
1:A:404:ARG:O	1:A:407:VAL:HG22	2.02	0.59
1:G:177:VAL:HG22	1:G:379:ILE:HD12	1.83	0.59
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.84	0.59
1:A:123:ALA:O	1:A:127:ALA:N	2.26	0.59
1:A:100:ILE:HD11	1:A:511:ALA:HA	1.84	0.59
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.84	0.59
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.84	0.59
1:I:232:GLU:HB3	1:I:309:LEU:HB2	1.84	0.59
1:A:232:GLU:HB3	1:A:309:LEU:HB2	1.84	0.59
1:L:177:VAL:HG22	1:L:379:ILE:HD12	1.83	0.59
1:A:411:VAL:HG21	1:A:494:LEU:HD13	1.85	0.59
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.84	0.59
1:C:177:VAL:HG22	1:C:379:ILE:HD12	1.83	0.59
1:A:296:THR:OG1	1:A:319:GLN:N	2.36	0.59
1:A:177:VAL:HG22	1:A:379:ILE:HD12	1.83	0.59
1:D:177:VAL:HG22	1:D:379:ILE:HD12	1.83	0.59
1:F:177:VAL:HG22	1:F:379:ILE:HD12	1.83	0.59
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.84	0.59
1:A:219:PHE:HB2	1:A:245:LYS:HZ3	1.66	0.59
1:I:177:VAL:HG22	1:I:379:ILE:HD12	1.83	0.59
1:N:177:VAL:HG22	1:N:379:ILE:HD12	1.83	0.59
1:J:177:VAL:HG22	1:J:379:ILE:HD12	1.83	0.59
1:A:413:ALA:HB1	1:A:488:MET:HB2	1.83	0.59
1:B:177:VAL:HG22	1:B:379:ILE:HD12	1.83	0.59
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.84	0.59
1:M:177:VAL:HG22	1:M:379:ILE:HD12	1.83	0.58
1:A:120:ILE:O	1:A:123:ALA:N	2.36	0.58
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.84	0.58
1:A:31:LEU:O	1:A:457:ASN:ND2	2.37	0.58
1:E:177:VAL:HG22	1:E:379:ILE:HD12	1.83	0.58
1:I:31:LEU:O	1:I:457:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:O	1:A:135:SER:N	2.35	0.58
1:A:149:THR:HB	1:A:154:SER:HA	1.86	0.58
1:N:31:LEU:O	1:N:457:ASN:ND2	2.37	0.58
1:A:177:VAL:HG13	1:A:379:ILE:HB	1.86	0.58
1:A:230:ILE:HD11	1:A:258:ALA:HA	1.84	0.58
1:F:31:LEU:O	1:F:457:ASN:ND2	2.37	0.58
1:A:255:GLU:HA	1:A:259:LEU:HD13	1.85	0.58
1:A:203:TYR:OH	1:A:267:MET:HA	2.03	0.58
1:A:220:ILE:HG23	1:A:248:LEU:HG	1.85	0.58
1:A:282:GLY:O	1:A:285:ARG:NE	2.36	0.58
1:A:463:SER:O	1:A:467:ASN:HB2	2.04	0.58
1:A:523:ASP:OD1	1:A:524:LEU:N	2.37	0.58
1:G:31:LEU:O	1:G:457:ASN:ND2	2.37	0.57
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.85	0.57
1:A:128:VAL:HG21	1:A:505:GLN:HE21	1.70	0.57
1:E:31:LEU:O	1:E:457:ASN:ND2	2.37	0.57
1:H:31:LEU:O	1:H:457:ASN:ND2	2.37	0.57
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.86	0.57
1:A:284:ARG:HG3	1:A:285:ARG:HH22	1.68	0.57
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.86	0.57
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.86	0.57
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.57
1:I:128:VAL:HG21	1:I:505:GLN:HE21	1.70	0.57
1:A:199:TYR:HB3	1:A:325:ILE:HG12	1.85	0.57
1:G:128:VAL:HG21	1:G:505:GLN:HE21	1.70	0.57
1:H:128:VAL:HG21	1:H:505:GLN:HE21	1.70	0.57
1:M:31:LEU:O	1:M:457:ASN:ND2	2.37	0.57
1:A:219:PHE:HE2	1:A:245:LYS:HB3	1.69	0.57
1:L:31:LEU:O	1:L:457:ASN:ND2	2.37	0.57
1:A:353:ILE:HG22	1:A:365:LEU:HB3	1.86	0.57
1:D:31:LEU:O	1:D:457:ASN:ND2	2.37	0.57
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.57
1:A:346:VAL:O	1:A:350:ARG:N	2.29	0.57
1:K:31:LEU:O	1:K:457:ASN:ND2	2.37	0.57
1:A:414:GLY:H	1:A:494:LEU:HA	1.69	0.57
1:A:206:ASN:OD1	1:A:213:VAL:HA	2.04	0.57
1:A:511:ALA:O	1:A:515:ILE:N	2.32	0.57
1:B:31:LEU:O	1:B:457:ASN:ND2	2.37	0.57
1:C:31:LEU:O	1:C:457:ASN:ND2	2.37	0.57
1:C:124:VAL:HG21	1:C:508:ALA:HB2	1.87	0.57
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:128:VAL:HG21	1:J:505:GLN:HE21	1.70	0.57
1:A:219:PHE:O	1:A:245:LYS:NZ	2.37	0.57
1:B:128:VAL:HG21	1:B:505:GLN:HE21	1.70	0.57
1:K:124:VAL:HG21	1:K:508:ALA:HB2	1.87	0.57
1:A:326:ASN:N	1:A:329:THR:O	2.38	0.57
1:D:124:VAL:HG21	1:D:508:ALA:HB2	1.87	0.56
1:J:124:VAL:HG21	1:J:508:ALA:HB2	1.87	0.56
1:L:124:VAL:HG21	1:L:508:ALA:HB2	1.87	0.56
1:M:124:VAL:HG21	1:M:508:ALA:HB2	1.87	0.56
1:A:421:ARG:NH1	1:A:472:GLY:O	2.38	0.56
1:B:124:VAL:HG21	1:B:508:ALA:HB2	1.87	0.56
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.86	0.56
1:E:124:VAL:HG21	1:E:508:ALA:HB2	1.87	0.56
1:J:31:LEU:O	1:J:457:ASN:ND2	2.37	0.56
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.86	0.56
1:A:126:VAL:HG11	1:A:429:LEU:HD22	1.87	0.56
1:A:102:GLU:OE1	1:A:445:ARG:NH2	2.38	0.56
1:A:206:ASN:H	1:A:213:VAL:HG23	1.69	0.56
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.56
1:D:128:VAL:HG21	1:D:505:GLN:HE21	1.70	0.56
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.86	0.56
1:L:128:VAL:HG21	1:L:505:GLN:HE21	1.70	0.56
1:A:178:GLU:HB2	1:A:378:VAL:HA	1.88	0.56
1:A:305:ILE:HG23	1:A:307:MET:HG2	1.87	0.56
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.86	0.56
1:E:128:VAL:HG21	1:E:505:GLN:HE21	1.70	0.56
1:I:124:VAL:HG21	1:I:508:ALA:HB2	1.87	0.56
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.87	0.56
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.56
1:A:219:PHE:HB2	1:A:245:LYS:NZ	2.21	0.56
1:A:353:ILE:HA	1:A:356:ALA:HB2	1.88	0.56
1:A:398:ASP:OD1	1:A:399:ALA:N	2.39	0.56
1:A:414:GLY:HA3	1:A:493:ILE:HG22	1.88	0.56
1:M:128:VAL:HG21	1:M:505:GLN:HE21	1.70	0.56
1:N:128:VAL:HG21	1:N:505:GLN:HE21	1.70	0.56
1:A:230:ILE:CD1	1:A:258:ALA:HA	2.35	0.56
1:G:124:VAL:HG21	1:G:508:ALA:HB2	1.87	0.56
1:A:178:GLU:OE2	1:A:333:ILE:HG21	2.05	0.56
1:A:216:GLU:O	1:A:245:LYS:HE2	2.06	0.56
1:A:160:LYS:O	1:A:164:GLU:HG2	2.06	0.56
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:VAL:HG21	1:F:505:GLN:HE21	1.70	0.56
1:F:124:VAL:HG21	1:F:508:ALA:HB2	1.87	0.56
1:H:124:VAL:HG21	1:H:508:ALA:HB2	1.87	0.56
1:N:124:VAL:HG21	1:N:508:ALA:HB2	1.87	0.56
1:K:128:VAL:HG21	1:K:505:GLN:HE21	1.70	0.56
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.56
1:A:199:TYR:CE1	1:A:327:LYS:HA	2.41	0.56
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.88	0.55
1:A:420:ILE:HD11	1:A:448:GLU:HA	1.88	0.55
1:C:128:VAL:HG21	1:C:505:GLN:HE21	1.70	0.55
1:A:279:PRO:O	1:A:285:ARG:NE	2.39	0.55
1:A:199:TYR:CZ	1:A:205:ILE:HD11	2.42	0.55
1:A:116:LEU:O	1:A:119:GLY:N	2.39	0.55
1:A:194:GLN:HA	1:A:330:THR:O	2.06	0.55
1:A:219:PHE:CE2	1:A:245:LYS:HB3	2.42	0.55
1:A:122:LYS:NZ	1:A:430:ARG:O	2.34	0.55
1:A:313:THR:H	1:A:316:ASP:HB2	1.72	0.55
1:A:115:ASP:OD2	1:A:436:GLN:N	2.40	0.55
1:B:177:VAL:HG13	1:B:379:ILE:HB	1.89	0.55
1:J:177:VAL:HG13	1:J:379:ILE:HB	1.89	0.55
1:A:175:ILE:HB	1:A:377:ALA:HB2	1.89	0.55
1:F:177:VAL:HG13	1:F:379:ILE:HB	1.89	0.55
1:N:177:VAL:HG13	1:N:379:ILE:HB	1.89	0.55
1:A:87:ASP:OD1	1:A:88:GLY:N	2.36	0.55
1:A:32:GLY:O	1:A:35:GLY:N	2.40	0.54
1:A:128:VAL:HG21	1:A:505:GLN:HE21	1.73	0.54
1:E:177:VAL:HG13	1:E:379:ILE:HB	1.90	0.54
1:M:177:VAL:HG13	1:M:379:ILE:HB	1.90	0.54
1:A:240:VAL:HG23	1:A:245:LYS:HE3	1.90	0.54
1:A:284:ARG:HG3	1:A:285:ARG:NH2	2.22	0.54
1:A:87:ASP:OD1	1:A:88:GLY:N	2.37	0.54
1:A:40:LEU:HD11	1:A:56:VAL:HG22	1.89	0.54
1:A:177:VAL:HG13	1:A:379:ILE:HB	1.90	0.54
1:C:177:VAL:HG13	1:C:379:ILE:HB	1.89	0.54
1:I:177:VAL:HG13	1:I:379:ILE:HB	1.90	0.54
1:A:319:GLN:O	1:A:336:VAL:HG23	2.07	0.54
1:H:177:VAL:HG13	1:H:379:ILE:HB	1.89	0.54
1:K:177:VAL:HG13	1:K:379:ILE:HB	1.90	0.54
1:A:135:SER:HA	1:A:412:VAL:HG12	1.89	0.54
1:A:131:LEU:HG	1:A:422:VAL:HG11	1.89	0.54
1:A:431:GLY:H	1:A:437:ASN:ND2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:O	1:A:284:ARG:NH1	2.40	0.54
1:A:353:ILE:HD13	1:A:365:LEU:HG	1.90	0.54
1:D:177:VAL:HG13	1:D:379:ILE:HB	1.90	0.54
1:A:27:VAL:HA	1:A:30:THR:HG22	1.90	0.54
1:A:294:THR:O	1:A:337:GLY:HA3	2.08	0.54
1:G:177:VAL:HG13	1:G:379:ILE:HB	1.90	0.54
1:L:177:VAL:HG13	1:L:379:ILE:HB	1.90	0.54
1:A:19:GLY:HA2	1:A:67:GLU:OE2	2.08	0.54
1:A:7:LYS:CB	1:A:12:ALA:HB2	2.38	0.53
1:A:195:PHE:CZ	1:A:330:THR:HB	2.43	0.53
1:A:220:ILE:CB	1:A:318:GLY:O	2.52	0.53
1:A:435:ASP:HA	1:A:438:VAL:HG22	1.91	0.53
1:A:123:ALA:HB2	1:A:440:ILE:HG23	1.88	0.53
1:A:7:LYS:HB3	1:A:12:ALA:HB2	1.90	0.53
1:A:176:THR:O	1:A:377:ALA:CB	2.45	0.53
1:M:323:VAL:HG12	1:M:332:ILE:HA	1.91	0.53
1:A:348:GLN:O	1:A:351:GLN:HB3	2.09	0.53
1:E:323:VAL:HG12	1:E:332:ILE:HA	1.91	0.53
1:A:401:HIS:O	1:A:404:ARG:HB3	2.09	0.53
1:A:247:LEU:O	1:A:274:ALA:N	2.39	0.53
1:A:107:VAL:HG21	1:A:113:PRO:HG3	1.90	0.53
1:J:323:VAL:HG12	1:J:332:ILE:HA	1.91	0.53
1:N:323:VAL:HG12	1:N:332:ILE:HA	1.91	0.53
1:A:201:SER:H	1:A:204:PHE:HE2	1.54	0.53
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.91	0.53
1:L:323:VAL:HG12	1:L:332:ILE:HA	1.91	0.52
1:A:186:GLU:H	1:A:380:LYS:HB2	1.74	0.52
1:D:323:VAL:HG12	1:D:332:ILE:HA	1.91	0.52
1:F:323:VAL:HG12	1:F:332:ILE:HA	1.91	0.52
1:I:323:VAL:HG12	1:I:332:ILE:HA	1.91	0.52
1:A:219:PHE:CE2	1:A:245:LYS:HB2	2.45	0.52
1:B:323:VAL:HG12	1:B:332:ILE:HA	1.91	0.52
1:C:323:VAL:HG12	1:C:332:ILE:HA	1.91	0.52
1:K:323:VAL:HG12	1:K:332:ILE:HA	1.91	0.52
1:A:250:ILE:HA	1:A:276:VAL:O	2.09	0.52
1:A:64:ASP:HB3	1:A:67:GLU:HB3	1.91	0.52
1:H:323:VAL:HG12	1:H:332:ILE:HA	1.91	0.52
1:A:230:ILE:HD12	1:A:231:ARG:N	2.23	0.52
1:A:461:GLU:OE1	1:A:464:VAL:N	2.39	0.52
1:A:323:VAL:HG12	1:A:332:ILE:HA	1.91	0.52
1:E:24:ALA:O	1:E:28:LYS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:323:VAL:HG12	1:G:332:ILE:HA	1.91	0.52
1:M:24:ALA:O	1:M:28:LYS:HB3	2.10	0.52
1:A:219:PHE:CD2	1:A:245:LYS:HE2	2.45	0.52
1:A:135:SER:HA	1:A:412:VAL:HG12	1.92	0.52
1:A:421:ARG:NH1	1:A:472:GLY:O	2.42	0.52
1:F:349:ILE:HG12	1:F:368:ARG:HH21	1.75	0.52
1:N:349:ILE:HG12	1:N:368:ARG:HH21	1.75	0.52
1:A:126:VAL:HG11	1:A:429:LEU:CD2	2.38	0.52
1:A:77:VAL:HG21	1:A:510:VAL:CG1	2.40	0.52
1:A:193:MET:HE3	1:A:292:ILE:HG12	1.91	0.52
1:F:24:ALA:O	1:F:28:LYS:HB3	2.10	0.52
1:N:24:ALA:O	1:N:28:LYS:HB3	2.10	0.52
1:A:230:ILE:HD12	1:A:231:ARG:N	2.24	0.52
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.90	0.52
1:D:187:LEU:HD13	1:D:379:ILE:HG12	1.92	0.52
1:D:24:ALA:O	1:D:28:LYS:HB3	2.10	0.52
1:A:296:THR:HB	1:A:318:GLY:HA3	1.91	0.52
1:A:363:GLU:HA	1:A:366:GLN:HE21	1.75	0.52
1:E:349:ILE:HG12	1:E:368:ARG:HH21	1.75	0.52
1:H:349:ILE:HG12	1:H:368:ARG:HH21	1.75	0.52
1:L:24:ALA:O	1:L:28:LYS:HB3	2.10	0.52
1:L:187:LEU:HD13	1:L:379:ILE:HG12	1.92	0.52
1:M:349:ILE:HG12	1:M:368:ARG:HH21	1.75	0.52
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.92	0.52
1:A:303:GLU:N	1:A:303:GLU:OE1	2.37	0.52
1:A:240:VAL:CG2	1:A:245:LYS:HE3	2.40	0.52
1:D:349:ILE:HG12	1:D:368:ARG:HH21	1.75	0.51
1:G:349:ILE:HG12	1:G:368:ARG:HH21	1.75	0.51
1:M:187:LEU:HD13	1:M:379:ILE:HG12	1.92	0.51
1:A:162:ILE:H	1:A:162:ILE:HD12	1.75	0.51
1:A:156:GLU:O	1:A:160:LYS:HD3	2.09	0.51
1:A:421:ARG:NH1	1:A:472:GLY:O	2.43	0.51
1:C:187:LEU:HD13	1:C:379:ILE:HG12	1.92	0.51
1:E:187:LEU:HD13	1:E:379:ILE:HG12	1.92	0.51
1:J:187:LEU:HD13	1:J:379:ILE:HG12	1.92	0.51
1:B:24:ALA:O	1:B:28:LYS:HB3	2.10	0.51
1:B:187:LEU:HD13	1:B:379:ILE:HG12	1.92	0.51
1:C:24:ALA:O	1:C:28:LYS:HB3	2.10	0.51
1:G:24:ALA:O	1:G:28:LYS:HB3	2.10	0.51
1:G:171:LYS:O	1:G:404:ARG:NH1	2.44	0.51
1:H:24:ALA:O	1:H:28:LYS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:GLU:O	1:H:261:THR:OG1	2.26	0.51
1:H:171:LYS:O	1:H:404:ARG:NH1	2.44	0.51
1:K:24:ALA:O	1:K:28:LYS:HB3	2.10	0.51
1:L:349:ILE:HG12	1:L:368:ARG:HH21	1.75	0.51
1:A:340:ALA:O	1:A:343:GLN:HG3	2.10	0.51
1:A:42:LYS:HZ3	1:A:44:PHE:HE1	1.56	0.51
1:A:234:LEU:HD13	1:A:237:LEU:HD11	1.92	0.51
1:F:171:LYS:O	1:F:404:ARG:NH1	2.44	0.51
1:I:349:ILE:HG12	1:I:368:ARG:HH21	1.75	0.51
1:I:171:LYS:O	1:I:404:ARG:NH1	2.44	0.51
1:J:24:ALA:O	1:J:28:LYS:HB3	2.10	0.51
1:K:187:LEU:HD13	1:K:379:ILE:HG12	1.92	0.51
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.92	0.51
1:A:171:LYS:O	1:A:404:ARG:NH1	2.44	0.51
1:E:171:LYS:O	1:E:404:ARG:NH1	2.44	0.51
1:G:257:GLU:O	1:G:261:THR:OG1	2.26	0.51
1:M:171:LYS:O	1:M:404:ARG:NH1	2.44	0.51
1:N:171:LYS:O	1:N:404:ARG:NH1	2.44	0.51
1:A:219:PHE:HD2	1:A:245:LYS:HE2	1.75	0.51
1:A:254:VAL:HG12	1:A:259:LEU:HD12	1.93	0.51
1:A:213:VAL:O	1:A:324:VAL:HA	2.11	0.51
1:A:504:LEU:O	1:A:507:ALA:N	2.44	0.51
1:J:349:ILE:HG12	1:J:368:ARG:HH21	1.75	0.51
1:A:288:MET:HG2	1:A:368:ARG:NH1	2.26	0.51
1:A:349:ILE:HG12	1:A:368:ARG:HH21	1.75	0.51
1:A:187:LEU:HD13	1:A:379:ILE:HG12	1.93	0.51
1:A:234:LEU:HD23	1:A:235:PRO:HD3	1.93	0.51
1:I:187:LEU:HD13	1:I:379:ILE:HG12	1.92	0.51
1:I:24:ALA:O	1:I:28:LYS:HB3	2.10	0.51
1:K:349:ILE:HG12	1:K:368:ARG:HH21	1.75	0.51
1:A:165:ALA:HB1	1:A:175:ILE:HD12	1.92	0.51
1:A:187:LEU:HD13	1:A:379:ILE:HG12	1.92	0.51
1:A:24:ALA:O	1:A:28:LYS:HB3	2.10	0.51
1:A:281:PHE:HA	1:A:285:ARG:HE	1.76	0.51
1:B:349:ILE:HG12	1:B:368:ARG:HH21	1.75	0.51
1:I:281:PHE:HA	1:I:285:ARG:HE	1.76	0.51
1:A:223:ALA:HB3	1:A:249:ILE:HG23	1.91	0.51
1:A:122:LYS:HD3	1:A:440:ILE:HD11	1.92	0.51
1:A:387:VAL:HG23	1:A:390:LYS:HZ1	1.75	0.51
1:F:187:LEU:HD13	1:F:379:ILE:HG12	1.92	0.51
1:F:281:PHE:HA	1:F:285:ARG:HE	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:187:LEU:HD13	1:N:379:ILE:HG12	1.92	0.51
1:A:213:VAL:HG22	1:A:325:ILE:HB	1.92	0.51
1:A:224:ASP:O	1:A:225:LYS:HD2	2.11	0.51
1:A:254:VAL:HG23	1:A:259:LEU:HB3	1.92	0.51
1:D:171:LYS:O	1:D:404:ARG:NH1	2.44	0.50
1:L:171:LYS:O	1:L:404:ARG:NH1	2.44	0.50
1:N:281:PHE:HA	1:N:285:ARG:HE	1.76	0.50
1:A:390:LYS:O	1:A:393:LYS:HB3	2.11	0.50
1:A:388:GLU:O	1:A:392:LYS:N	2.37	0.50
1:A:505:GLN:O	1:A:508:ALA:N	2.44	0.50
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.93	0.50
1:C:349:ILE:HG12	1:C:368:ARG:HH21	1.75	0.50
1:D:421:ARG:NH1	1:D:472:GLY:O	2.45	0.50
1:H:187:LEU:HD13	1:H:379:ILE:HG12	1.92	0.50
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.93	0.50
1:G:187:LEU:HD13	1:G:379:ILE:HG12	1.92	0.50
1:J:171:LYS:O	1:J:404:ARG:NH1	2.44	0.50
1:K:281:PHE:HA	1:K:285:ARG:HE	1.76	0.50
1:L:421:ARG:NH1	1:L:472:GLY:O	2.45	0.50
1:A:34:LYS:HG3	1:A:458:CYS:SG	2.50	0.50
1:B:171:LYS:O	1:B:404:ARG:NH1	2.44	0.50
1:C:281:PHE:HA	1:C:285:ARG:HE	1.76	0.50
1:C:171:LYS:O	1:C:404:ARG:NH1	2.44	0.50
1:D:281:PHE:HA	1:D:285:ARG:HE	1.76	0.50
1:E:421:ARG:NH1	1:E:472:GLY:O	2.45	0.50
1:K:171:LYS:O	1:K:404:ARG:NH1	2.44	0.50
1:L:281:PHE:HA	1:L:285:ARG:HE	1.76	0.50
1:M:421:ARG:NH1	1:M:472:GLY:O	2.45	0.50
1:A:389:MET:O	1:A:392:LYS:N	2.43	0.50
1:A:249:ILE:N	1:A:274:ALA:O	2.31	0.50
1:A:421:ARG:NH1	1:A:472:GLY:O	2.45	0.50
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.93	0.50
1:H:421:ARG:NH1	1:H:472:GLY:O	2.45	0.50
1:I:421:ARG:NH1	1:I:472:GLY:O	2.45	0.50
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.93	0.50
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.93	0.50
1:A:288:MET:HA	1:A:291:ASP:OD2	2.12	0.50
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.93	0.50
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.93	0.50
1:G:421:ARG:NH1	1:G:472:GLY:O	2.45	0.50
1:A:109:ALA:HB2	1:J:109:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:421:ARG:NH1	1:K:472:GLY:O	2.45	0.50
1:A:141:SER:O	1:A:144:ILE:HG22	2.12	0.50
1:A:257:GLU:O	1:A:261:THR:HB	2.11	0.50
1:A:295:LEU:O	1:A:337:GLY:N	2.42	0.50
1:A:342:ILE:O	1:A:346:VAL:HG23	2.12	0.50
1:C:421:ARG:NH1	1:C:472:GLY:O	2.45	0.50
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.93	0.50
1:G:281:PHE:HA	1:G:285:ARG:HE	1.76	0.50
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.93	0.50
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.93	0.50
1:H:281:PHE:HA	1:H:285:ARG:HE	1.76	0.50
1:F:109:ALA:HB2	1:L:109:ALA:HB2	1.93	0.50
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.93	0.50
1:A:10:ASN:O	1:A:14:VAL:HG22	2.12	0.50
1:A:23:LEU:HD13	1:A:60:ILE:HD11	1.93	0.50
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.93	0.50
1:B:109:ALA:HB2	1:I:109:ALA:HB2	1.94	0.50
1:A:115:ASP:OD2	1:A:433:ASN:ND2	2.32	0.50
1:A:254:VAL:HG21	1:A:275:ALA:HB1	1.93	0.50
1:A:213:VAL:HG22	1:A:325:ILE:CG2	2.42	0.50
1:F:421:ARG:NH1	1:F:472:GLY:O	2.45	0.49
1:G:109:ALA:HB2	1:K:109:ALA:HB2	1.93	0.49
1:A:155:ASP:OD1	1:A:156:GLU:N	2.40	0.49
1:A:24:ALA:O	1:A:28:LYS:HG2	2.11	0.49
1:A:435:ASP:O	1:A:438:VAL:HG12	2.12	0.49
1:N:247:LEU:O	1:N:273:VAL:HA	2.13	0.49
1:N:421:ARG:NH1	1:N:472:GLY:O	2.45	0.49
1:A:228:SER:OG	1:A:255:GLU:O	2.29	0.49
1:A:223:ALA:HB3	1:A:227:ILE:HD11	1.93	0.49
1:A:94:VAL:HG12	1:A:449:ALA:HB1	1.95	0.49
1:B:421:ARG:NH1	1:B:472:GLY:O	2.45	0.49
1:D:22:VAL:HG11	1:D:62:LEU:HD21	1.95	0.49
1:E:22:VAL:HG11	1:E:62:LEU:HD21	1.95	0.49
1:E:281:PHE:HA	1:E:285:ARG:HE	1.76	0.49
1:F:247:LEU:O	1:F:273:VAL:HA	2.13	0.49
1:G:247:LEU:O	1:G:273:VAL:HA	2.13	0.49
1:H:247:LEU:O	1:H:273:VAL:HA	2.13	0.49
1:J:281:PHE:HA	1:J:285:ARG:HE	1.76	0.49
1:J:421:ARG:NH1	1:J:472:GLY:O	2.45	0.49
1:L:22:VAL:HG11	1:L:62:LEU:HD21	1.95	0.49
1:M:22:VAL:HG11	1:M:62:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD21	1:A:438:VAL:HG23	1.94	0.49
1:A:365:LEU:HA	1:A:368:ARG:HB2	1.93	0.49
1:A:247:LEU:O	1:A:273:VAL:HA	2.13	0.49
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.94	0.49
1:E:247:LEU:O	1:E:273:VAL:HA	2.13	0.49
1:M:281:PHE:HA	1:M:285:ARG:HE	1.76	0.49
1:A:196:ASP:HA	1:A:329:THR:HG23	1.94	0.49
1:B:281:PHE:HA	1:B:285:ARG:HE	1.77	0.49
1:C:109:ALA:HB2	1:H:109:ALA:HB2	1.94	0.49
1:I:247:LEU:O	1:I:273:VAL:HA	2.13	0.49
1:M:247:LEU:O	1:M:273:VAL:HA	2.13	0.49
1:A:350:ARG:O	1:A:353:ILE:HG12	2.12	0.49
1:A:39:VAL:HG22	1:A:49:ILE:HG12	1.95	0.49
1:A:326:ASN:HB3	1:A:329:THR:H	1.77	0.49
1:F:22:VAL:HG11	1:F:62:LEU:HD21	1.95	0.49
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.93	0.49
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.95	0.49
1:A:257:GLU:O	1:A:261:THR:CB	2.61	0.49
1:A:314:LEU:HD22	1:A:317:LEU:HD11	1.95	0.49
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.95	0.49
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.95	0.49
1:A:441:LYS:O	1:A:445:ARG:HG3	2.13	0.49
1:A:368:ARG:O	1:A:371:LYS:HB3	2.13	0.49
1:A:496:PRO:HD2	1:A:499:VAL:HG11	1.94	0.49
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.93	0.49
1:B:247:LEU:O	1:B:273:VAL:HA	2.13	0.49
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.93	0.49
1:D:247:LEU:O	1:D:273:VAL:HA	2.13	0.49
1:J:247:LEU:O	1:J:273:VAL:HA	2.13	0.49
1:L:247:LEU:O	1:L:273:VAL:HA	2.13	0.49
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.95	0.49
1:A:420:ILE:CD1	1:A:448:GLU:HA	2.42	0.49
1:D:109:ALA:HB2	1:N:109:ALA:HB2	1.94	0.49
1:A:222:LEU:O	1:A:301:ILE:HG22	2.13	0.49
1:C:247:LEU:O	1:C:273:VAL:HA	2.13	0.48
1:A:219:PHE:CD1	1:A:319:GLN:HB2	2.48	0.48
1:A:213:VAL:H	1:A:325:ILE:HG22	1.78	0.48
1:J:248:LEU:HD22	1:J:323:VAL:HG21	1.95	0.48
1:K:247:LEU:O	1:K:273:VAL:HA	2.13	0.48
1:A:205:ILE:HG23	1:A:212:ALA:O	2.13	0.48
1:A:338:GLU:O	1:A:342:ILE:N	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.94	0.48
1:B:248:LEU:HD22	1:B:323:VAL:HG21	1.95	0.48
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.96	0.48
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.96	0.48
1:E:248:LEU:HD22	1:E:323:VAL:HG21	1.95	0.48
1:A:10:ASN:O	1:A:13:GLY:N	2.46	0.48
1:A:463:SER:O	1:A:467:ASN:CB	2.62	0.48
1:A:219:PHE:HB3	1:A:317:LEU:HD13	1.94	0.48
1:A:289:LEU:HD12	1:A:290:GLN:N	2.27	0.48
1:A:135:SER:HA	1:A:412:VAL:HG12	1.95	0.48
1:A:248:LEU:HD22	1:A:323:VAL:HG21	1.95	0.48
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.96	0.48
1:K:40:LEU:HD13	1:K:59:GLU:HG3	1.96	0.48
1:L:40:LEU:HD13	1:L:59:GLU:HG3	1.96	0.48
1:M:40:LEU:HD13	1:M:59:GLU:HG3	1.96	0.48
1:M:519:CYS:HB3	1:N:38:VAL:HG22	1.95	0.48
1:H:38:VAL:HG22	1:N:519:CYS:HB3	1.95	0.48
1:A:157:THR:O	1:A:160:LYS:HB3	2.13	0.48
1:A:519:CYS:SG	1:A:520:MET:N	2.86	0.48
1:A:339:GLU:HA	1:A:342:ILE:HG22	1.95	0.48
1:A:487:ASN:O	1:A:491:MET:HG3	2.12	0.48
1:A:169:VAL:HG12	1:A:173:GLY:HA3	1.96	0.48
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.48	0.48
1:A:421:ARG:NE	1:A:474:GLY:O	2.46	0.48
1:A:458:CYS:SG	2:A:602:HOH:O	2.60	0.48
1:B:22:VAL:HG11	1:B:62:LEU:HD21	1.95	0.48
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.96	0.48
1:F:40:LEU:HD13	1:F:59:GLU:HG3	1.96	0.48
1:G:40:LEU:HD13	1:G:59:GLU:HG3	1.96	0.48
1:G:22:VAL:HG11	1:G:62:LEU:HD21	1.95	0.48
1:H:40:LEU:HD13	1:H:59:GLU:HG3	1.96	0.48
1:M:248:LEU:HD22	1:M:323:VAL:HG21	1.95	0.48
1:A:253:ASP:OD1	1:A:254:VAL:N	2.45	0.48
1:A:166:MET:O	1:A:170:GLY:N	2.47	0.48
1:A:247:LEU:HD13	1:A:248:LEU:N	2.28	0.48
1:A:179:ASP:HB2	1:A:389:MET:HE2	1.95	0.48
1:A:194:GLN:HG3	1:A:331:THR:HG22	1.95	0.48
1:A:308:GLU:OE2	1:A:311:LYS:NZ	2.38	0.48
1:H:22:VAL:HG11	1:H:62:LEU:HD21	1.95	0.48
1:I:248:LEU:HD22	1:I:323:VAL:HG21	1.95	0.48
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:LEU:HD13	1:N:59:GLU:HG3	1.96	0.48
1:A:261:THR:O	1:A:264:VAL:HB	2.12	0.48
1:A:289:LEU:HA	1:A:292:ILE:HG22	1.95	0.48
1:A:16:MET:O	1:A:19:GLY:N	2.45	0.48
1:F:248:LEU:HD22	1:F:323:VAL:HG21	1.95	0.48
1:H:519:CYS:HB3	1:I:38:VAL:HG22	1.96	0.48
1:N:248:LEU:HD22	1:N:323:VAL:HG21	1.95	0.48
1:A:220:ILE:H	1:A:319:GLN:HA	1.78	0.48
1:A:260:ALA:O	1:A:264:VAL:HG23	2.14	0.48
1:A:358:SER:O	1:A:362:ARG:HG3	2.14	0.48
1:A:232:GLU:OE2	1:A:308:GLU:HG3	2.13	0.48
1:I:40:LEU:HD13	1:I:59:GLU:HG3	1.96	0.48
1:L:519:CYS:HB3	1:M:38:VAL:HG22	1.94	0.48
1:A:113:PRO:C	1:A:115:ASP:H	2.16	0.48
1:A:362:ARG:O	1:A:366:GLN:NE2	2.47	0.48
1:A:122:LYS:NZ	1:A:430:ARG:O	2.33	0.48
1:C:248:LEU:HD22	1:C:323:VAL:HG21	1.95	0.48
1:H:77:VAL:HG12	1:H:506:TYR:HB3	1.96	0.48
1:K:248:LEU:HD22	1:K:323:VAL:HG21	1.95	0.48
1:A:221:LEU:O	1:A:248:LEU:O	2.32	0.48
1:A:121:ASP:O	1:A:125:THR:HG22	2.14	0.48
1:A:240:VAL:O	1:A:244:GLY:N	2.45	0.48
1:A:476:TYR:HH	1:A:485:TYR:HD2	1.61	0.48
1:A:38:VAL:HG22	1:G:519:CYS:HB3	1.96	0.48
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.96	0.48
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.96	0.48
1:J:270:ILE:HG22	1:J:271:VAL:HG23	1.96	0.48
1:J:217:SER:N	1:J:321:LYS:O	2.46	0.48
1:J:40:LEU:HD13	1:J:59:GLU:HG3	1.96	0.48
1:A:167:ASP:OD1	1:A:168:LYS:N	2.46	0.48
1:B:217:SER:N	1:B:321:LYS:O	2.46	0.47
1:B:40:LEU:HD13	1:B:59:GLU:HG3	1.96	0.47
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.96	0.47
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.96	0.47
1:I:77:VAL:HG12	1:I:506:TYR:HB3	1.96	0.47
1:L:270:ILE:HG22	1:L:271:VAL:HG23	1.96	0.47
1:M:270:ILE:HG22	1:M:271:VAL:HG23	1.96	0.47
1:M:217:SER:N	1:M:321:LYS:O	2.46	0.47
1:A:230:ILE:HG23	1:A:257:GLU:CG	2.43	0.47
1:A:303:GLU:OE1	1:A:303:GLU:N	2.44	0.47
1:A:219:PHE:HA	1:A:319:GLN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:HG12	1:A:393:LYS:NZ	2.29	0.47
1:A:200:LEU:HG	1:A:276:VAL:HA	1.96	0.47
1:A:221:LEU:HD22	1:A:236:VAL:HG11	1.97	0.47
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.96	0.47
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.96	0.47
1:F:77:VAL:HG12	1:F:506:TYR:HB3	1.96	0.47
1:N:257:GLU:O	1:N:261:THR:OG1	2.26	0.47
1:N:77:VAL:HG12	1:N:506:TYR:HB3	1.96	0.47
1:A:288:MET:O	1:A:291:ASP:N	2.48	0.47
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.96	0.47
1:D:221:LEU:HD22	1:D:236:VAL:HG11	1.97	0.47
1:D:248:LEU:HD22	1:D:323:VAL:HG21	1.95	0.47
1:E:217:SER:N	1:E:321:LYS:O	2.46	0.47
1:I:221:LEU:HD22	1:I:236:VAL:HG11	1.97	0.47
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.96	0.47
1:A:115:ASP:OD2	1:A:436:GLN:HG3	2.14	0.47
1:A:194:GLN:HE21	1:A:329:THR:HG21	1.79	0.47
1:A:237:LEU:HD21	1:A:247:LEU:HG	1.96	0.47
1:A:225:LYS:HE3	1:A:227:ILE:HG12	1.96	0.47
1:A:213:VAL:N	1:A:325:ILE:HG22	2.29	0.47
1:A:22:VAL:HG11	1:A:62:LEU:HD21	1.95	0.47
1:B:221:LEU:HD22	1:B:236:VAL:HG11	1.97	0.47
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.96	0.47
1:C:221:LEU:HD22	1:C:236:VAL:HG11	1.97	0.47
1:I:270:ILE:HG22	1:I:271:VAL:HG23	1.96	0.47
1:J:77:VAL:HG12	1:J:506:TYR:HB3	1.96	0.47
1:K:221:LEU:HD22	1:K:236:VAL:HG11	1.97	0.47
1:L:221:LEU:HD22	1:L:236:VAL:HG11	1.97	0.47
1:L:248:LEU:HD22	1:L:323:VAL:HG21	1.95	0.47
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.96	0.47
1:I:22:VAL:HG11	1:I:62:LEU:HD21	1.95	0.47
1:J:221:LEU:HD22	1:J:236:VAL:HG11	1.97	0.47
1:K:254:VAL:HG12	1:K:259:LEU:HB2	1.97	0.47
1:A:296:THR:O	1:A:336:VAL:HB	2.15	0.47
1:A:352:GLN:HA	1:A:355:GLU:OE2	2.15	0.47
1:A:155:ASP:HB2	1:A:395:ARG:HH12	1.79	0.47
1:A:77:VAL:HG21	1:A:510:VAL:HG13	1.97	0.47
1:A:519:CYS:HB3	1:B:38:VAL:HG22	1.96	0.47
1:C:254:VAL:HG12	1:C:259:LEU:HB2	1.97	0.47
1:G:221:LEU:HD22	1:G:236:VAL:HG11	1.97	0.47
1:L:254:VAL:HG12	1:L:259:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:221:LEU:HD22	1:M:236:VAL:HG11	1.97	0.47
1:A:339:GLU:O	1:A:343:GLN:CB	2.60	0.47
1:A:197:ARG:NE	1:A:278:ALA:O	2.48	0.47
1:A:403:THR:HA	1:A:406:ALA:HB3	1.96	0.47
1:A:478:TYR:HB2	1:A:485:TYR:CE1	2.49	0.47
1:A:42:LYS:HZ3	1:A:44:PHE:HB3	1.80	0.47
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.97	0.47
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.97	0.47
1:E:109:ALA:HB2	1:M:109:ALA:HB2	1.96	0.47
1:E:221:LEU:HD22	1:E:236:VAL:HG11	1.97	0.47
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.96	0.47
1:H:221:LEU:HD22	1:H:236:VAL:HG11	1.97	0.47
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.97	0.47
1:I:519:CYS:HB3	1:J:38:VAL:HG22	1.96	0.47
1:G:248:LEU:HD22	1:G:323:VAL:HG21	1.95	0.47
1:J:519:CYS:HB3	1:K:38:VAL:HG22	1.95	0.47
1:N:270:ILE:HG22	1:N:271:VAL:HG23	1.96	0.47
1:A:391:GLU:OE2	1:A:395:ARG:NE	2.27	0.47
1:A:419:LEU:HD22	1:A:504:LEU:HD12	1.95	0.47
1:A:461:GLU:OE1	1:A:463:SER:N	2.48	0.47
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.96	0.47
1:H:248:LEU:HD22	1:H:323:VAL:HG21	1.95	0.47
1:H:270:ILE:HG22	1:H:271:VAL:HG23	1.96	0.47
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.97	0.47
1:N:221:LEU:HD22	1:N:236:VAL:HG11	1.97	0.47
1:A:356:ALA:O	1:A:362:ARG:NH2	2.48	0.47
1:A:361:ASP:O	1:A:365:LEU:HD23	2.14	0.47
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.97	0.47
1:F:221:LEU:HD22	1:F:236:VAL:HG11	1.97	0.47
1:M:513:LEU:HB3	1:N:49:ILE:HD13	1.97	0.47
1:A:389:MET:O	1:A:392:LYS:N	2.48	0.47
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.96	0.47
1:E:435:ASP:HA	1:E:438:VAL:HG22	1.97	0.47
1:E:77:VAL:HG12	1:E:506:TYR:HB3	1.96	0.47
1:E:519:CYS:HB3	1:F:38:VAL:HG22	1.96	0.47
1:H:217:SER:N	1:H:321:LYS:O	2.46	0.47
1:K:77:VAL:HG12	1:K:506:TYR:HB3	1.96	0.47
1:A:228:SER:C	1:A:257:GLU:HB3	2.35	0.47
1:B:519:CYS:HB3	1:C:38:VAL:HG22	1.96	0.46
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.96	0.46
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:435:ASP:HA	1:M:438:VAL:HG22	1.97	0.46
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.97	0.46
1:A:7:LYS:HB3	1:A:12:ALA:HB2	1.95	0.46
1:A:115:ASP:OD2	1:A:435:ASP:HB2	2.15	0.46
1:A:129:GLU:O	1:A:132:LYS:N	2.48	0.46
1:A:149:THR:HG21	1:A:156:GLU:HA	1.97	0.46
1:A:230:ILE:O	1:A:234:LEU:N	2.42	0.46
1:A:193:MET:SD	1:A:332:ILE:HD13	2.55	0.46
1:A:364:LYS:O	1:A:367:GLU:HB2	2.15	0.46
1:D:519:CYS:HB3	1:E:38:VAL:HG22	1.96	0.46
1:G:217:SER:N	1:G:321:LYS:O	2.46	0.46
1:L:77:VAL:HG12	1:L:506:TYR:HB3	1.96	0.46
1:M:77:VAL:HG12	1:M:506:TYR:HB3	1.96	0.46
1:A:28:LYS:HD3	1:A:453:GLN:NE2	2.30	0.46
1:A:226:LYS:HD3	1:A:255:GLU:OE2	2.15	0.46
1:A:194:GLN:HE21	1:A:329:THR:HG21	1.79	0.46
1:A:496:PRO:O	1:A:499:VAL:HG12	2.15	0.46
1:D:435:ASP:HA	1:D:438:VAL:HG22	1.97	0.46
1:F:435:ASP:HA	1:F:438:VAL:HG22	1.97	0.46
1:L:435:ASP:HA	1:L:438:VAL:HG22	1.97	0.46
1:N:435:ASP:HA	1:N:438:VAL:HG22	1.97	0.46
1:A:236:VAL:HG22	1:A:312:ALA:O	2.15	0.46
1:A:124:VAL:O	1:A:127:ALA:N	2.48	0.46
1:G:254:VAL:HG12	1:G:259:LEU:HB2	1.97	0.46
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.97	0.46
1:A:265:ASN:O	1:A:269:GLY:N	2.48	0.46
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.97	0.46
1:A:223:ALA:O	1:A:250:ILE:C	2.53	0.46
1:A:251:ALA:O	1:A:278:ALA:N	2.30	0.46
1:A:219:PHE:HB2	1:A:247:LEU:HD23	1.98	0.46
1:G:435:ASP:HA	1:G:438:VAL:HG22	1.97	0.46
1:I:254:VAL:HG12	1:I:259:LEU:HB2	1.97	0.46
1:A:203:TYR:CD2	1:A:263:VAL:HG13	2.51	0.46
1:A:369:VAL:O	1:A:373:ALA:N	2.40	0.46
1:A:199:TYR:CE1	1:A:327:LYS:HA	2.50	0.46
1:A:16:MET:SD	1:A:514:MET:HG3	2.56	0.46
1:A:230:ILE:O	1:A:234:LEU:HG	2.16	0.46
1:A:257:GLU:O	1:A:261:THR:OG1	2.26	0.46
1:A:200:LEU:HD23	1:A:200:LEU:H	1.81	0.46
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.97	0.46
1:A:197:ARG:HE	1:A:279:PRO:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:HB1	1:A:89:THR:HG23	1.97	0.46
1:H:435:ASP:HA	1:H:438:VAL:HG22	1.97	0.46
1:L:217:SER:N	1:L:321:LYS:O	2.46	0.46
1:L:78:ALA:HB1	1:L:89:THR:HG23	1.97	0.46
1:A:20:VAL:O	1:A:23:LEU:N	2.49	0.46
1:A:144:ILE:HA	1:A:147:VAL:HG12	1.97	0.46
1:A:259:LEU:O	1:A:263:VAL:HG23	2.16	0.46
1:G:78:ALA:HB1	1:G:89:THR:HG23	1.97	0.46
1:I:197:ARG:HE	1:I:279:PRO:HA	1.81	0.46
1:K:78:ALA:HB1	1:K:89:THR:HG23	1.97	0.46
1:A:180:GLY:H	1:A:389:MET:CE	2.29	0.46
1:A:185:ASP:CA	1:A:382:GLY:H	2.29	0.46
1:A:510:VAL:O	1:A:514:MET:N	2.44	0.46
1:D:213:VAL:HB	1:D:325:ILE:HB	1.99	0.45
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.96	0.45
1:D:78:ALA:HB1	1:D:89:THR:HG23	1.97	0.45
1:H:197:ARG:HE	1:H:279:PRO:HA	1.81	0.45
1:I:257:GLU:O	1:I:261:THR:OG1	2.26	0.45
1:I:78:ALA:HB1	1:I:89:THR:HG23	1.97	0.45
1:K:197:ARG:HE	1:K:279:PRO:HA	1.81	0.45
1:L:213:VAL:HB	1:L:325:ILE:HB	1.99	0.45
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.56	0.45
1:A:257:GLU:O	1:A:261:THR:N	2.49	0.45
1:A:359:ASP:HA	1:A:362:ARG:HE	1.80	0.45
1:B:197:ARG:HE	1:B:279:PRO:HA	1.81	0.45
1:C:197:ARG:HE	1:C:279:PRO:HA	1.81	0.45
1:C:78:ALA:HB1	1:C:89:THR:HG23	1.97	0.45
1:D:217:SER:N	1:D:321:LYS:O	2.46	0.45
1:G:197:ARG:HE	1:G:279:PRO:HA	1.81	0.45
1:H:78:ALA:HB1	1:H:89:THR:HG23	1.97	0.45
1:A:239:ALA:O	1:A:242:LYS:HG3	2.16	0.45
1:A:197:ARG:O	1:A:330:THR:OG1	2.24	0.45
1:A:85:ALA:HB1	1:A:499:VAL:HG23	1.99	0.45
1:A:19:GLY:HA2	1:A:67:GLU:OE2	2.17	0.45
1:A:363:GLU:O	1:A:367:GLU:HG3	2.17	0.45
1:B:78:ALA:HB1	1:B:89:THR:HG23	1.97	0.45
1:C:213:VAL:HB	1:C:325:ILE:HB	1.99	0.45
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.99	0.45
1:J:197:ARG:HE	1:J:279:PRO:HA	1.81	0.45
1:J:213:VAL:HB	1:J:325:ILE:HB	1.99	0.45
1:K:213:VAL:HB	1:K:325:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:519:CYS:HB3	1:L:38:VAL:HG22	1.97	0.45
1:A:487:ASN:HB3	1:A:490:ASP:HB2	1.97	0.45
1:A:100:ILE:O	1:A:103:GLY:N	2.45	0.45
1:A:343:GLN:O	1:A:347:ALA:N	2.32	0.45
1:A:417:VAL:HG21	1:A:488:MET:HE3	1.98	0.45
1:A:213:VAL:HB	1:A:325:ILE:HB	1.99	0.45
1:A:435:ASP:HA	1:A:438:VAL:HG22	1.97	0.45
1:B:213:VAL:HB	1:B:325:ILE:HB	1.99	0.45
1:B:435:ASP:HA	1:B:438:VAL:HG22	1.97	0.45
1:I:217:SER:N	1:I:321:LYS:O	2.46	0.45
1:I:213:VAL:HB	1:I:325:ILE:HB	1.99	0.45
1:J:435:ASP:HA	1:J:438:VAL:HG22	1.97	0.45
1:J:78:ALA:HB1	1:J:89:THR:HG23	1.97	0.45
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.99	0.45
1:A:193:MET:HE3	1:A:292:ILE:HG21	1.98	0.45
1:A:194:GLN:HG2	1:A:331:THR:HB	1.98	0.45
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.99	0.45
1:E:213:VAL:HB	1:E:325:ILE:HB	1.99	0.45
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.99	0.45
1:K:435:ASP:HA	1:K:438:VAL:HG22	1.97	0.45
1:M:213:VAL:HB	1:M:325:ILE:HB	1.99	0.45
1:N:197:ARG:HE	1:N:279:PRO:HA	1.81	0.45
1:A:232:GLU:OE2	1:A:310:GLU:HG2	2.16	0.45
1:A:193:MET:HB3	1:A:332:ILE:HB	1.97	0.45
1:A:161:LEU:O	1:A:164:GLU:HB2	2.16	0.45
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.99	0.45
1:C:435:ASP:HA	1:C:438:VAL:HG22	1.97	0.45
1:I:435:ASP:HA	1:I:438:VAL:HG22	1.97	0.45
1:A:320:ALA:HA	1:A:334:ASP:O	2.17	0.45
1:A:414:GLY:N	1:A:494:LEU:HA	2.31	0.45
1:A:217:SER:N	1:A:321:LYS:O	2.46	0.45
1:E:78:ALA:HB1	1:E:89:THR:HG23	1.97	0.45
1:F:197:ARG:HE	1:F:279:PRO:HA	1.81	0.45
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.99	0.45
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.99	0.45
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.99	0.45
1:M:78:ALA:HB1	1:M:89:THR:HG23	1.97	0.45
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.99	0.45
1:A:176:THR:H	1:A:376:VAL:HG12	1.81	0.45
1:A:397:GLU:O	1:A:400:LEU:HB3	2.17	0.45
1:A:191:GLU:OE1	1:A:335:GLY:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:HA	1:A:296:THR:HG22	1.98	0.45
1:A:353:ILE:HA	1:A:365:LEU:HD11	1.97	0.45
1:D:197:ARG:HE	1:D:279:PRO:HA	1.81	0.45
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.99	0.45
1:F:78:ALA:HB1	1:F:89:THR:HG23	1.97	0.45
1:L:197:ARG:HE	1:L:279:PRO:HA	1.81	0.45
1:A:215:LEU:HB2	1:A:323:VAL:CG2	2.47	0.45
1:A:346:VAL:O	1:A:350:ARG:HG2	2.17	0.45
1:A:5:ASP:HB2	1:A:524:LEU:HD22	1.97	0.45
1:A:311:LYS:HD2	1:A:311:LYS:N	2.31	0.45
1:A:265:ASN:OD1	1:A:270:ILE:HB	2.17	0.45
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.99	0.45
1:F:513:LEU:HB3	1:G:49:ILE:HD13	1.99	0.45
1:G:213:VAL:HB	1:G:325:ILE:HB	1.99	0.45
1:H:213:VAL:HB	1:H:325:ILE:HB	1.99	0.45
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.99	0.45
1:H:49:ILE:HD13	1:N:513:LEU:HB3	1.99	0.45
1:N:78:ALA:HB1	1:N:89:THR:HG23	1.97	0.45
1:A:217:SER:HA	1:A:321:LYS:HA	1.99	0.45
1:A:186:GLU:OE1	1:A:187:LEU:N	2.50	0.45
1:A:346:VAL:HA	1:A:349:ILE:HG22	1.98	0.45
1:A:128:VAL:HG21	1:A:505:GLN:NE2	2.31	0.45
1:M:197:ARG:HE	1:M:279:PRO:HA	1.81	0.44
1:A:252:GLU:HB2	1:A:285:ARG:NH1	2.32	0.44
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.98	0.44
1:A:233:MET:O	1:A:237:LEU:HD12	2.18	0.44
1:A:346:VAL:O	1:A:349:ILE:HG22	2.18	0.44
1:A:264:VAL:HA	1:A:267:MET:HB3	1.98	0.44
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.99	0.44
1:D:222:LEU:HD23	1:D:250:ILE:HB	1.99	0.44
1:E:197:ARG:HE	1:E:279:PRO:HA	1.81	0.44
1:F:213:VAL:HB	1:F:325:ILE:HB	1.99	0.44
1:K:222:LEU:HD23	1:K:250:ILE:HB	1.99	0.44
1:L:222:LEU:HD23	1:L:250:ILE:HB	1.99	0.44
1:M:149:THR:HG22	1:M:156:GLU:HA	1.99	0.44
1:B:257:GLU:O	1:B:261:THR:OG1	2.26	0.44
1:D:149:THR:HG22	1:D:156:GLU:HA	1.99	0.44
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.99	0.44
1:L:149:THR:HG22	1:L:156:GLU:HA	1.99	0.44
1:N:106:ALA:HB3	1:N:116:LEU:HD21	1.99	0.44
1:N:213:VAL:HB	1:N:325:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HD2	1:A:246:PRO:O	2.17	0.44
1:A:359:ASP:OD1	1:A:362:ARG:NH1	2.50	0.44
1:A:66:PHE:CD1	1:A:520:MET:HE1	2.49	0.44
1:A:107:VAL:CG2	1:A:113:PRO:HG3	2.47	0.44
1:A:406:ALA:HA	1:A:496:PRO:HB3	1.98	0.44
1:C:222:LEU:HD23	1:C:250:ILE:HB	2.00	0.44
1:F:106:ALA:HB3	1:F:116:LEU:HD21	1.99	0.44
1:A:188:ASP:N	1:A:188:ASP:OD1	2.50	0.44
1:A:233:MET:SD	1:A:237:LEU:HD23	2.57	0.44
1:A:419:LEU:O	1:A:423:ALA:N	2.41	0.44
1:E:106:ALA:HB3	1:E:116:LEU:HD21	1.99	0.44
1:J:513:LEU:HB3	1:K:49:ILE:HD13	1.99	0.44
1:M:106:ALA:HB3	1:M:116:LEU:HD21	1.99	0.44
1:N:149:THR:HG22	1:N:156:GLU:HA	1.99	0.44
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.99	0.44
1:A:30:THR:HB	1:A:51:LYS:O	2.17	0.44
1:A:111:MET:SD	1:A:438:VAL:HG21	2.58	0.44
1:A:228:SER:HA	1:A:258:ALA:CB	2.46	0.44
1:A:174:VAL:HG11	1:A:376:VAL:HG22	2.00	0.44
1:A:205:ILE:HG12	1:A:211:GLY:O	2.18	0.44
1:A:295:LEU:HD12	1:A:296:THR:N	2.32	0.44
1:A:363:GLU:HA	1:A:366:GLN:HB3	2.00	0.44
1:A:513:LEU:HB3	1:B:49:ILE:HD13	1.99	0.44
1:E:149:THR:HG22	1:E:156:GLU:HA	1.99	0.44
1:G:222:LEU:HD23	1:G:250:ILE:HB	1.99	0.44
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.99	0.44
1:I:513:LEU:HB3	1:J:49:ILE:HD13	1.99	0.44
1:A:268:ARG:NH1	1:A:270:ILE:HG21	2.33	0.44
1:A:396:VAL:O	1:A:400:LEU:N	2.50	0.44
1:C:149:THR:HG22	1:C:156:GLU:HA	1.99	0.44
1:B:513:LEU:HB3	1:C:49:ILE:HD13	1.99	0.44
1:F:149:THR:HG22	1:F:156:GLU:HA	1.99	0.44
1:K:149:THR:HG22	1:K:156:GLU:HA	1.99	0.44
1:A:286:LYS:HD3	1:A:286:LYS:H	1.83	0.44
1:A:294:THR:HG21	1:A:342:ILE:HA	1.99	0.44
1:A:344:GLY:O	1:A:348:GLN:N	2.35	0.44
1:A:213:VAL:HG12	1:A:325:ILE:HB	1.99	0.44
1:A:301:ILE:HD13	1:A:309:LEU:HA	2.00	0.44
1:A:339:GLU:HA	1:A:342:ILE:HB	1.99	0.44
1:A:411:VAL:HG21	1:A:494:LEU:HB3	2.00	0.44
1:H:513:LEU:HB3	1:I:49:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:ALA:HB3	1:L:116:LEU:HD21	1.99	0.44
1:A:149:THR:CG2	1:A:156:GLU:HA	2.48	0.44
1:A:222:LEU:HD22	1:A:289:LEU:HD12	2.00	0.44
1:A:197:ARG:HH21	1:A:280:GLY:N	2.16	0.44
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.99	0.43
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.99	0.43
1:H:106:ALA:HB3	1:H:116:LEU:HD21	1.99	0.43
1:H:149:THR:HG22	1:H:156:GLU:HA	1.99	0.43
1:L:513:LEU:HB3	1:M:49:ILE:HD13	1.99	0.43
1:A:38:VAL:HG11	1:A:56:VAL:HG11	2.00	0.43
1:A:365:LEU:O	1:A:369:VAL:HG12	2.17	0.43
1:A:209:GLU:N	1:A:209:GLU:OE1	2.37	0.43
1:A:226:LYS:HD3	1:A:226:LYS:H	1.83	0.43
1:E:222:LEU:HD23	1:E:250:ILE:HB	1.99	0.43
1:D:513:LEU:HB3	1:E:49:ILE:HD13	1.99	0.43
1:G:149:THR:HG22	1:G:156:GLU:HA	1.99	0.43
1:M:222:LEU:HD23	1:M:250:ILE:HB	1.99	0.43
1:A:268:ARG:HB2	1:A:270:ILE:HG13	2.00	0.43
1:A:178:GLU:CD	1:A:322:ARG:HD3	2.39	0.43
1:A:378:VAL:CG2	1:A:380:LYS:HD3	2.47	0.43
1:A:381:VAL:HG11	1:A:393:LYS:N	2.34	0.43
1:A:288:MET:HE3	1:A:368:ARG:HH12	1.83	0.43
1:B:222:LEU:HD23	1:B:250:ILE:HB	2.00	0.43
1:A:49:ILE:HD13	1:G:513:LEU:HB3	1.99	0.43
1:J:222:LEU:HD23	1:J:250:ILE:HB	2.00	0.43
1:K:513:LEU:HB3	1:L:49:ILE:HD13	1.99	0.43
1:A:225:LYS:O	1:A:251:ALA:HB1	2.17	0.43
1:A:221:LEU:HD12	1:A:236:VAL:HG11	1.99	0.43
1:A:230:ILE:O	1:A:233:MET:N	2.50	0.43
1:A:285:ARG:O	1:A:288:MET:N	2.51	0.43
1:A:190:VAL:HG11	1:A:333:ILE:HG23	2.01	0.43
1:I:149:THR:HG22	1:I:156:GLU:HA	1.99	0.43
1:A:245:LYS:HG3	1:A:246:PRO:HD2	1.99	0.43
1:A:222:LEU:O	1:A:301:ILE:N	2.51	0.43
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.99	0.43
1:E:513:LEU:HB3	1:F:49:ILE:HD13	2.01	0.43
1:J:106:ALA:HB3	1:J:116:LEU:HD21	1.99	0.43
1:A:308:GLU:CD	1:A:309:LEU:N	2.72	0.43
1:A:389:MET:O	1:A:393:LYS:HG2	2.18	0.43
1:B:149:THR:HG22	1:B:156:GLU:HA	1.99	0.43
1:J:149:THR:HG22	1:J:156:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:OE2	1:A:322:ARG:NE	2.25	0.43
1:A:403:THR:O	1:A:407:VAL:HG13	2.18	0.43
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.75	0.43
1:A:177:VAL:HG12	1:A:393:LYS:HE2	2.00	0.43
1:A:149:THR:HG22	1:A:156:GLU:HA	1.99	0.43
1:C:431:GLY:H	1:C:437:ASN:ND2	2.17	0.43
1:D:20:VAL:O	1:D:24:ALA:HB3	2.18	0.43
1:I:322:ARG:O	1:I:333:ILE:HB	2.19	0.43
1:J:20:VAL:O	1:J:24:ALA:HB3	2.18	0.43
1:K:106:ALA:HB3	1:K:116:LEU:HD21	1.99	0.43
1:L:20:VAL:O	1:L:24:ALA:HB3	2.19	0.43
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.79	0.43
1:A:488:MET:HE3	1:A:493:ILE:HB	2.00	0.43
1:A:255:GLU:N	1:A:255:GLU:OE1	2.51	0.43
1:A:283:ASP:O	1:A:286:LYS:HG2	2.19	0.43
1:A:322:ARG:O	1:A:333:ILE:HB	2.19	0.43
1:B:20:VAL:O	1:B:24:ALA:HB3	2.18	0.43
1:B:431:GLY:H	1:B:437:ASN:ND2	2.17	0.43
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.99	0.43
1:J:322:ARG:O	1:J:333:ILE:HB	2.19	0.43
1:J:431:GLY:H	1:J:437:ASN:ND2	2.17	0.43
1:K:431:GLY:H	1:K:437:ASN:ND2	2.17	0.43
1:A:31:LEU:HD12	1:A:32:GLY:H	1.83	0.43
1:A:144:ILE:HG13	1:A:403:THR:HG23	2.01	0.43
1:A:265:ASN:O	1:A:270:ILE:HG13	2.19	0.43
1:A:278:ALA:HB1	1:A:289:LEU:HD21	2.00	0.43
1:A:431:GLY:H	1:A:437:ASN:ND2	2.17	0.43
1:C:513:LEU:HB3	1:D:49:ILE:HD13	2.00	0.43
1:F:431:GLY:H	1:F:437:ASN:ND2	2.17	0.43
1:G:322:ARG:O	1:G:333:ILE:HB	2.19	0.43
1:H:322:ARG:O	1:H:333:ILE:HB	2.19	0.43
1:I:431:GLY:H	1:I:437:ASN:ND2	2.17	0.43
1:A:237:LEU:HA	1:A:240:VAL:CG1	2.49	0.43
1:A:68:ASN:O	1:A:72:GLN:HG2	2.19	0.43
1:A:363:GLU:O	1:A:367:GLU:HG3	2.19	0.43
1:A:124:VAL:O	1:A:128:VAL:HG12	2.18	0.43
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.99	0.43
1:B:322:ARG:O	1:B:333:ILE:HB	2.19	0.43
1:I:106:ALA:HB3	1:I:116:LEU:HD21	1.99	0.43
1:I:20:VAL:O	1:I:24:ALA:HB3	2.18	0.43
1:K:20:VAL:O	1:K:24:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:431:GLY:H	1:L:437:ASN:ND2	2.17	0.43
1:M:20:VAL:O	1:M:24:ALA:HB3	2.18	0.43
1:N:431:GLY:H	1:N:437:ASN:ND2	2.17	0.43
1:A:174:VAL:HG21	1:A:194:GLN:CD	2.39	0.43
1:A:421:ARG:NH2	1:A:476:TYR:O	2.52	0.43
1:A:87:ASP:HB3	1:A:499:VAL:HG21	2.01	0.43
1:A:161:LEU:HD11	1:A:379:ILE:HG23	2.00	0.43
1:A:249:ILE:O	1:A:275:ALA:HA	2.19	0.43
1:C:20:VAL:O	1:C:24:ALA:HB3	2.19	0.42
1:D:431:GLY:H	1:D:437:ASN:ND2	2.17	0.42
1:E:20:VAL:O	1:E:24:ALA:HB3	2.18	0.42
1:F:322:ARG:O	1:F:333:ILE:HB	2.19	0.42
1:N:322:ARG:O	1:N:333:ILE:HB	2.19	0.42
1:A:144:ILE:HA	1:A:147:VAL:HG12	2.01	0.42
1:A:215:LEU:HB3	1:A:218:PRO:HB3	2.00	0.42
1:A:22:VAL:HG11	1:A:62:LEU:HD21	2.00	0.42
1:K:178:GLU:HG2	1:K:322:ARG:HH11	1.85	0.42
1:M:431:GLY:H	1:M:437:ASN:ND2	2.17	0.42
1:A:20:VAL:O	1:A:24:ALA:HB3	2.19	0.42
1:A:222:LEU:HD23	1:A:250:ILE:HB	1.99	0.42
1:C:178:GLU:HG2	1:C:322:ARG:HH11	1.85	0.42
1:E:240:VAL:HG21	1:E:247:LEU:HD22	2.02	0.42
1:M:240:VAL:HG21	1:M:247:LEU:HD22	2.02	0.42
1:A:247:LEU:HD13	1:A:248:LEU:N	2.34	0.42
1:B:178:GLU:HG2	1:B:322:ARG:HH11	1.85	0.42
1:D:240:VAL:HG21	1:D:247:LEU:HD22	2.02	0.42
1:E:431:GLY:H	1:E:437:ASN:ND2	2.17	0.42
1:F:20:VAL:O	1:F:24:ALA:HB3	2.18	0.42
1:F:222:LEU:HD23	1:F:250:ILE:HB	1.99	0.42
1:G:20:VAL:O	1:G:24:ALA:HB3	2.18	0.42
1:J:178:GLU:HG2	1:J:322:ARG:HH11	1.85	0.42
1:A:359:ASP:O	1:A:362:ARG:HB2	2.19	0.42
1:A:81:ALA:O	1:A:85:ALA:N	2.52	0.42
1:A:219:PHE:CD1	1:A:319:GLN:HG3	2.54	0.42
1:D:178:GLU:HG2	1:D:322:ARG:HH11	1.84	0.42
1:F:240:VAL:HG21	1:F:247:LEU:HD22	2.02	0.42
1:H:431:GLY:H	1:H:437:ASN:ND2	2.17	0.42
1:I:222:LEU:HD23	1:I:250:ILE:HB	1.99	0.42
1:L:240:VAL:HG21	1:L:247:LEU:HD22	2.02	0.42
1:L:178:GLU:HG2	1:L:322:ARG:HH11	1.85	0.42
1:N:20:VAL:O	1:N:24:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:LEU:HD23	1:N:250:ILE:HB	2.00	0.42
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.69	0.42
1:A:4:LYS:HD2	1:A:521:VAL:HG12	2.01	0.42
1:A:177:VAL:HG11	1:A:393:LYS:HG3	2.00	0.42
1:A:204:PHE:CE2	1:A:213:VAL:HG21	2.54	0.42
1:A:262:LEU:HD12	1:A:273:VAL:O	2.19	0.42
1:A:358:SER:HB3	1:A:361:ASP:OD2	2.20	0.42
1:G:431:GLY:H	1:G:437:ASN:ND2	2.17	0.42
1:H:20:VAL:O	1:H:24:ALA:HB3	2.18	0.42
1:H:5:ASP:HB2	1:H:524:LEU:HD23	2.02	0.42
1:K:217:SER:N	1:K:321:LYS:O	2.46	0.42
1:K:322:ARG:O	1:K:333:ILE:HB	2.19	0.42
1:N:240:VAL:HG21	1:N:247:LEU:HD22	2.02	0.42
1:N:217:SER:N	1:N:321:LYS:O	2.46	0.42
1:N:5:ASP:HB2	1:N:524:LEU:HD23	2.02	0.42
1:A:205:ILE:HA	1:A:213:VAL:HB	2.01	0.42
1:A:178:GLU:HG2	1:A:322:ARG:HH11	1.85	0.42
1:B:251:ALA:O	1:B:278:ALA:N	2.53	0.42
1:C:322:ARG:O	1:C:333:ILE:HB	2.19	0.42
1:F:251:ALA:O	1:F:278:ALA:N	2.53	0.42
1:F:5:ASP:HB2	1:F:524:LEU:HD23	2.02	0.42
1:N:251:ALA:O	1:N:278:ALA:N	2.53	0.42
1:N:178:GLU:HG2	1:N:322:ARG:HH11	1.85	0.42
1:A:235:PRO:O	1:A:238:GLU:HB2	2.20	0.42
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.82	0.42
1:A:383:ALA:HB1	1:A:388:GLU:CG	2.50	0.42
1:A:359:ASP:HA	1:A:362:ARG:NE	2.35	0.42
1:A:61:GLU:OE2	1:A:75:LYS:NZ	2.53	0.42
1:A:251:ALA:O	1:A:278:ALA:N	2.53	0.42
1:D:251:ALA:O	1:D:278:ALA:N	2.53	0.42
1:E:251:ALA:O	1:E:278:ALA:N	2.53	0.42
1:E:322:ARG:O	1:E:333:ILE:HB	2.19	0.42
1:G:5:ASP:HB2	1:G:524:LEU:HD23	2.02	0.42
1:H:178:GLU:HG2	1:H:322:ARG:HH11	1.85	0.42
1:I:178:GLU:HG2	1:I:322:ARG:HH11	1.85	0.42
1:J:251:ALA:O	1:J:278:ALA:N	2.53	0.42
1:K:399:ALA:O	1:K:403:THR:OG1	2.31	0.42
1:L:251:ALA:O	1:L:278:ALA:N	2.53	0.42
1:M:251:ALA:O	1:M:278:ALA:N	2.53	0.42
1:M:178:GLU:HG2	1:M:322:ARG:HH11	1.85	0.42
1:A:175:ILE:O	1:A:175:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:O	1:A:354:GLU:HG2	2.20	0.42
1:A:209:GLU:HG2	1:A:210:THR:N	2.34	0.42
1:E:178:GLU:HG2	1:E:322:ARG:HH11	1.85	0.42
1:F:217:SER:N	1:F:321:LYS:O	2.46	0.42
1:G:20:VAL:O	1:G:24:ALA:CB	2.68	0.42
1:G:251:ALA:O	1:G:278:ALA:N	2.53	0.42
1:G:178:GLU:HG2	1:G:322:ARG:HH11	1.85	0.42
1:G:421:ARG:NH2	1:G:469:VAL:O	2.53	0.42
1:H:20:VAL:O	1:H:24:ALA:CB	2.68	0.42
1:H:240:VAL:HG21	1:H:247:LEU:HD22	2.02	0.42
1:M:322:ARG:O	1:M:333:ILE:HB	2.19	0.42
1:A:245:LYS:HD2	1:A:245:LYS:C	2.40	0.42
1:A:365:LEU:HA	1:A:365:LEU:HD13	1.75	0.42
1:A:52:ASP:HB3	1:A:55:SER:HB2	2.02	0.42
1:A:132:LYS:HE2	1:A:409:GLU:OE1	2.20	0.42
1:A:252:GLU:O	1:A:277:LYS:HG3	2.20	0.42
1:A:152:ALA:HB2	1:A:399:ALA:HB2	2.00	0.42
1:A:27:VAL:HG13	1:A:90:THR:HG22	2.01	0.42
1:C:240:VAL:HG21	1:C:247:LEU:HD22	2.02	0.42
1:C:217:SER:N	1:C:321:LYS:O	2.46	0.42
1:E:464:VAL:HG11	1:N:467:ASN:HD22	1.85	0.42
1:F:178:GLU:HG2	1:F:322:ARG:HH11	1.85	0.42
1:F:20:VAL:O	1:F:24:ALA:CB	2.68	0.42
1:G:240:VAL:HG21	1:G:247:LEU:HD22	2.02	0.42
1:H:251:ALA:O	1:H:278:ALA:N	2.53	0.42
1:H:421:ARG:NH2	1:H:469:VAL:O	2.53	0.42
1:I:251:ALA:O	1:I:278:ALA:N	2.53	0.42
1:I:5:ASP:HB2	1:I:524:LEU:HD23	2.02	0.42
1:K:240:VAL:HG21	1:K:247:LEU:HD22	2.02	0.42
1:N:20:VAL:O	1:N:24:ALA:CB	2.68	0.42
1:A:390:LYS:HD3	1:A:393:LYS:HD3	2.01	0.42
1:A:27:VAL:HG21	1:A:57:ALA:HB2	2.02	0.42
1:A:64:ASP:HB3	1:A:67:GLU:CB	2.50	0.42
1:A:247:LEU:HD13	1:A:248:LEU:N	2.35	0.42
1:A:341:ALA:O	1:A:345:ARG:N	2.51	0.42
1:E:5:ASP:HB2	1:E:524:LEU:HD23	2.02	0.41
1:M:5:ASP:HB2	1:M:524:LEU:HD23	2.02	0.41
1:A:285:ARG:NE	1:A:285:ARG:HA	2.34	0.41
1:A:213:VAL:HG22	1:A:325:ILE:CB	2.50	0.41
1:A:239:ALA:HA	1:A:242:LYS:HE3	2.01	0.41
1:A:195:PHE:HB2	1:A:279:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:HE	1:A:369:VAL:HG21	1.84	0.41
1:A:226:LYS:O	1:A:226:LYS:HG2	2.20	0.41
1:A:338:GLU:HG3	1:A:340:ALA:H	1.84	0.41
1:A:5:ASP:HB2	1:A:524:LEU:HD23	2.02	0.41
1:D:322:ARG:O	1:D:333:ILE:HB	2.19	0.41
1:A:247:LEU:O	1:A:274:ALA:HB3	2.20	0.41
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.83	0.41
1:A:301:ILE:HG23	1:A:307:MET:HG3	2.02	0.41
1:A:325:ILE:HG13	1:A:326:ASN:O	2.19	0.41
1:A:15:LYS:O	1:A:67:GLU:HA	2.20	0.41
1:A:295:LEU:HD13	1:A:332:ILE:HD13	2.02	0.41
1:A:465:VAL:O	1:A:468:THR:N	2.53	0.41
1:A:20:VAL:O	1:A:24:ALA:CB	2.68	0.41
1:E:421:ARG:NH2	1:E:469:VAL:O	2.53	0.41
1:I:20:VAL:O	1:I:24:ALA:CB	2.68	0.41
1:L:322:ARG:O	1:L:333:ILE:HB	2.19	0.41
1:M:421:ARG:NH2	1:M:469:VAL:O	2.53	0.41
1:A:178:GLU:HG2	1:A:322:ARG:HH11	1.85	0.41
1:A:221:LEU:O	1:A:248:LEU:CA	2.67	0.41
1:A:242:LYS:NZ	1:A:314:LEU:HD11	2.35	0.41
1:A:162:ILE:HD11	1:A:396:VAL:HG23	2.03	0.41
1:A:240:VAL:HG21	1:A:247:LEU:HD22	2.02	0.41
1:A:464:VAL:HG11	1:K:467:ASN:HD22	1.86	0.41
1:A:22:VAL:HG11	1:A:62:LEU:HD21	2.03	0.41
1:A:265:ASN:OD1	1:A:270:ILE:HD11	2.20	0.41
1:A:346:VAL:O	1:A:350:ARG:HG2	2.20	0.41
1:A:262:LEU:HD11	1:A:275:ALA:HB2	2.02	0.41
1:A:352:GLN:OE1	1:A:365:LEU:HD13	2.20	0.41
1:A:99:ILE:O	1:A:103:GLY:N	2.54	0.41
1:B:240:VAL:HG21	1:B:247:LEU:HD22	2.02	0.41
1:C:251:ALA:O	1:C:278:ALA:N	2.53	0.41
1:E:20:VAL:O	1:E:24:ALA:CB	2.68	0.41
1:C:467:ASN:HD22	1:I:464:VAL:HG11	1.86	0.41
1:A:177:VAL:HG22	1:A:379:ILE:CG2	2.50	0.41
1:A:116:LEU:HD23	1:A:439:GLY:HA2	2.03	0.41
1:A:169:VAL:CG1	1:A:173:GLY:HA3	2.50	0.41
1:A:476:TYR:HA	1:A:486:GLY:O	2.20	0.41
1:A:467:ASN:HD22	1:K:464:VAL:HG11	1.86	0.41
1:H:399:ALA:O	1:H:403:THR:OG1	2.31	0.41
1:J:240:VAL:HG21	1:J:247:LEU:HD22	2.02	0.41
1:K:251:ALA:O	1:K:278:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:20:VAL:O	1:M:24:ALA:CB	2.68	0.41
1:A:92:ALA:HB2	1:A:503:ALA:HA	2.01	0.41
1:G:388:GLU:O	1:G:392:LYS:CB	2.69	0.41
1:H:388:GLU:O	1:H:392:LYS:CB	2.69	0.41
1:I:240:VAL:HG21	1:I:247:LEU:HD22	2.02	0.41
1:A:169:VAL:HG22	1:A:173:GLY:HA3	2.03	0.41
1:A:352:GLN:HA	1:A:355:GLU:OE2	2.20	0.41
1:B:5:ASP:HB2	1:B:524:LEU:HD23	2.02	0.41
1:C:388:GLU:O	1:C:392:LYS:CB	2.69	0.41
1:C:464:VAL:HG11	1:I:467:ASN:HD22	1.86	0.41
1:J:5:ASP:HB2	1:J:524:LEU:HD23	2.02	0.41
1:K:20:VAL:O	1:K:24:ALA:CB	2.68	0.41
1:K:388:GLU:O	1:K:392:LYS:CB	2.69	0.41
1:L:5:ASP:HB2	1:L:524:LEU:HD23	2.02	0.41
1:N:388:GLU:O	1:N:392:LYS:CB	2.69	0.41
1:A:175:ILE:HB	1:A:377:ALA:CB	2.50	0.41
1:A:213:VAL:HB	1:A:325:ILE:HG13	2.03	0.41
1:A:205:ILE:HD12	1:A:205:ILE:H	1.85	0.41
1:A:309:LEU:O	1:A:312:ALA:N	2.45	0.41
1:C:20:VAL:O	1:C:24:ALA:CB	2.68	0.41
1:F:388:GLU:O	1:F:392:LYS:CB	2.69	0.41
1:J:20:VAL:O	1:J:24:ALA:CB	2.68	0.41
1:A:421:ARG:NH2	1:A:469:VAL:O	2.53	0.41
1:B:20:VAL:O	1:B:24:ALA:CB	2.68	0.41
1:B:464:VAL:HG11	1:J:467:ASN:HD22	1.86	0.41
1:C:5:ASP:HB2	1:C:524:LEU:HD23	2.02	0.41
1:D:20:VAL:O	1:D:24:ALA:CB	2.68	0.41
1:D:5:ASP:HB2	1:D:524:LEU:HD23	2.02	0.41
1:E:467:ASN:HD22	1:N:464:VAL:HG11	1.86	0.41
1:K:5:ASP:HB2	1:K:524:LEU:HD23	2.02	0.41
1:L:20:VAL:O	1:L:24:ALA:CB	2.68	0.41
1:A:22:VAL:CG1	1:A:62:LEU:HD11	2.51	0.41
1:A:248:LEU:HA	1:A:248:LEU:HD13	1.87	0.41
1:A:376:VAL:HG12	1:A:377:ALA:N	2.33	0.41
1:A:423:ALA:HB2	1:A:447:MET:HB2	2.03	0.41
1:A:321:LYS:HG2	1:A:322:ARG:HH11	1.86	0.41
1:A:42:LYS:NZ	1:A:44:PHE:HE1	2.19	0.41
1:A:488:MET:SD	1:A:493:ILE:HD11	2.61	0.41
1:A:411:VAL:HG23	1:A:495:ASP:O	2.21	0.41
1:A:40:LEU:HD21	1:A:56:VAL:HA	2.02	0.41
1:A:283:ASP:O	1:A:285:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:O	1:A:392:LYS:CB	2.69	0.41
1:F:352:GLN:OE1	1:F:368:ARG:NH2	2.53	0.41
1:I:421:ARG:NH2	1:I:469:VAL:O	2.53	0.41
1:B:467:ASN:HD22	1:J:464:VAL:HG11	1.86	0.41
1:D:388:GLU:O	1:D:392:LYS:CB	2.69	0.40
1:I:388:GLU:O	1:I:392:LYS:CB	2.69	0.40
1:K:339:GLU:O	1:K:343:GLN:CB	2.70	0.40
1:A:207:LYS:HE3	1:A:210:THR:OG1	2.20	0.40
1:A:263:VAL:O	1:A:267:MET:HB3	2.22	0.40
1:A:42:LYS:NZ	1:A:44:PHE:HB3	2.36	0.40
1:A:347:ALA:O	1:A:351:GLN:HG2	2.21	0.40
1:B:388:GLU:O	1:B:392:LYS:CB	2.69	0.40
1:C:339:GLU:O	1:C:343:GLN:CB	2.70	0.40
1:J:388:GLU:O	1:J:392:LYS:CB	2.69	0.40
1:L:388:GLU:O	1:L:392:LYS:CB	2.69	0.40
1:A:301:ILE:HD13	1:A:301:ILE:HA	1.96	0.40
1:A:193:MET:HG3	1:A:371:LYS:NZ	2.36	0.40
1:A:252:GLU:HB2	1:A:285:ARG:HH11	1.86	0.40
1:A:232:GLU:O	1:A:309:LEU:HD12	2.20	0.40
1:C:102:GLU:HB2	1:C:442:VAL:HG13	2.04	0.40
1:H:339:GLU:O	1:H:343:GLN:CB	2.70	0.40
1:D:467:ASN:HD22	1:H:464:VAL:HG11	1.86	0.40
1:K:102:GLU:HB2	1:K:442:VAL:HG13	2.04	0.40
1:G:464:VAL:HG11	1:L:467:ASN:HD22	1.86	0.40
1:A:221:LEU:O	1:A:248:LEU:C	2.60	0.40
1:A:349:ILE:O	1:A:353:ILE:HG23	2.20	0.40
1:A:320:ALA:HB1	1:A:333:ILE:O	2.21	0.40
1:A:64:ASP:O	1:A:67:GLU:HB3	2.21	0.40
1:A:78:ALA:O	1:A:89:THR:OG1	2.36	0.40
1:A:18:ARG:HG3	1:A:67:GLU:HG2	2.03	0.40
1:A:324:VAL:HG22	1:A:331:THR:OG1	2.21	0.40
1:F:421:ARG:NH2	1:F:469:VAL:O	2.53	0.40
1:G:339:GLU:O	1:G:343:GLN:CB	2.70	0.40
1:G:352:GLN:OE1	1:G:368:ARG:NH2	2.53	0.40
1:K:158:VAL:HG13	1:K:396:VAL:HG22	2.04	0.40
1:L:102:GLU:HB2	1:L:442:VAL:HG13	2.04	0.40
1:L:158:VAL:HG13	1:L:396:VAL:HG22	2.04	0.40
1:M:339:GLU:O	1:M:343:GLN:CB	2.70	0.40
1:M:388:GLU:O	1:M:392:LYS:CB	2.69	0.40
1:A:254:VAL:HG13	1:A:258:ALA:CB	2.52	0.40
1:C:158:VAL:HG13	1:C:396:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLU:HB2	1:D:442:VAL:HG13	2.04	0.40
1:D:158:VAL:HG13	1:D:396:VAL:HG22	2.04	0.40
1:E:339:GLU:O	1:E:343:GLN:CB	2.70	0.40
1:N:421:ARG:NH2	1:N:469:VAL:O	2.53	0.40
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.77	0.40
1:A:78:ALA:HB1	1:A:89:THR:HG23	2.03	0.40
1:A:131:LEU:HA	1:A:131:LEU:HD23	1.79	0.40
1:A:220:ILE:HG22	1:A:248:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-B	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-C	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-D	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-E	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-F	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-G	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-H	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-I	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-J	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-K	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-L	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-M	522/524 (100%)	506 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-N	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	2-A	522/524 (100%)	445 (85%)	77 (15%)	0	100	100
1	3-A	522/524 (100%)	452 (87%)	70 (13%)	0	100	100
1	4-A	522/524 (100%)	468 (90%)	54 (10%)	0	100	100
All	All	8874/8908 (100%)	8449 (95%)	425 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	404/404 (100%)	404 (100%)	0	100	100
1	1-B	404/404 (100%)	404 (100%)	0	100	100
1	1-C	404/404 (100%)	404 (100%)	0	100	100
1	1-D	404/404 (100%)	404 (100%)	0	100	100
1	1-E	404/404 (100%)	404 (100%)	0	100	100
1	1-F	404/404 (100%)	404 (100%)	0	100	100
1	1-G	404/404 (100%)	404 (100%)	0	100	100
1	1-H	404/404 (100%)	404 (100%)	0	100	100
1	1-I	404/404 (100%)	404 (100%)	0	100	100
1	1-J	404/404 (100%)	404 (100%)	0	100	100
1	1-K	404/404 (100%)	404 (100%)	0	100	100
1	1-L	404/404 (100%)	404 (100%)	0	100	100
1	1-M	404/404 (100%)	404 (100%)	0	100	100
1	1-N	404/404 (100%)	404 (100%)	0	100	100
1	2-A	404/404 (100%)	400 (99%)	4 (1%)	80	91
1	3-A	404/404 (100%)	403 (100%)	1 (0%)	94	99
1	4-A	404/404 (100%)	400 (99%)	4 (1%)	80	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6868/6868 (100%)	6859 (100%)	9 (0%)	95 99

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2-A	242	LYS
1	2-A	245	LYS
1	2-A	327	LYS
1	2-A	445	ARG
1	3-A	225	LYS
1	4-A	226	LYS
1	4-A	277	LYS
1	4-A	284	ARG
1	4-A	390	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	37	ASN
1	1-A	505	GLN
1	1-B	37	ASN
1	1-B	505	GLN
1	1-C	37	ASN
1	1-C	505	GLN
1	1-D	37	ASN
1	1-D	505	GLN
1	1-E	37	ASN
1	1-E	505	GLN
1	1-F	37	ASN
1	1-F	505	GLN
1	1-G	37	ASN
1	1-G	505	GLN
1	1-H	37	ASN
1	1-H	505	GLN
1	1-I	37	ASN
1	1-I	505	GLN
1	1-J	37	ASN
1	1-J	505	GLN
1	1-K	37	ASN
1	1-K	505	GLN
1	1-L	37	ASN

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Mol	Chain	Res	Type
1	1-L	505	GLN
1	1-M	37	ASN
1	1-M	505	GLN
1	1-N	37	ASN
1	1-N	505	GLN
1	2-A	146	GLN
1	2-A	437	ASN
1	2-A	505	GLN
1	3-A	453	GLN
1	3-A	505	GLN
1	4-A	37	ASN
1	4-A	453	GLN
1	4-A	505	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.