W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Jun 5, 2023 – 04:12 PM JST

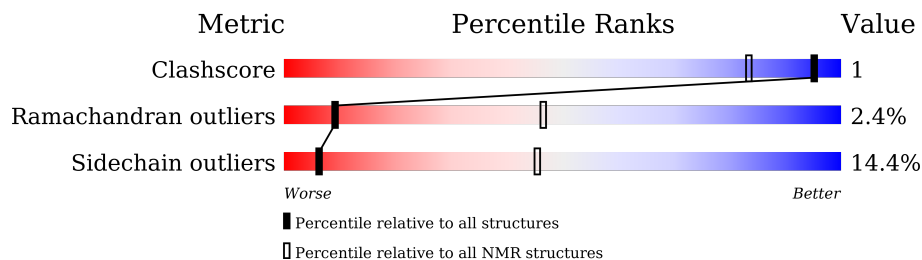|		
PDB ID	:	5X29
BMRB ID	:	36049
Title	:	NMR structure of the SARS Coronavirus E protein pentameric ion channel
Authors	:	Torres, J.; Surya, W.; Li, Y.
Deposited on	:	2017-01-31

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 19%.

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	Percentile Ranks	Value
Clashscore		1
Ramachandran outliers		2.4%
Sidechain outliers		14.4%

Worse *Better*

∎ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	81	62% · 10% · 28%
1	B	81	64% · 7% · 28%
1	C	81	60% · 11% · 28%
1	D	81	63% · 9% · 28%
1	E	81	60% · 11% · 28%

2 Ensemble composition and analysis ⓘ

This entry contains 16 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:65, B:8-B:65, C:8-C:65, D:8-D:65, E:8-E:65 (290)	2.34	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 9 single-model clusters were found.

Cluster number	Models
1	1, 4, 10, 11, 12
2	6, 13
Single-model clusters	2; 3; 5; 7; 8; 9; 14; 15; 16

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 4710 atoms, of which 2475 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope small membrane protein.

Mol	Chain	Residues	Atoms					Trace
1	A	58	Total	C	H	N	O	0
			942	301	495	70	76	
1	B	58	Total	C	H	N	O	0
			942	301	495	70	76	
1	C	58	Total	C	H	N	O	0
			942	301	495	70	76	
1	D	58	Total	C	H	N	O	0
			942	301	495	70	76	
1	E	58	Total	C	H	N	O	0
			942	301	495	70	76	

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P59637
A	-14	HIS	-	expression tag	UNP P59637
A	-13	HIS	-	expression tag	UNP P59637
A	-12	HIS	-	expression tag	UNP P59637
A	-11	HIS	-	expression tag	UNP P59637
A	-10	HIS	-	expression tag	UNP P59637
A	-9	HIS	-	expression tag	UNP P59637
A	-8	SER	-	expression tag	UNP P59637
A	-7	SER	-	expression tag	UNP P59637
A	-6	GLY	-	expression tag	UNP P59637
A	-5	VAL	-	expression tag	UNP P59637
A	-4	ASP	-	expression tag	UNP P59637
A	-3	LEU	-	expression tag	UNP P59637
A	-2	GLY	-	expression tag	UNP P59637
A	-1	THR	-	expression tag	UNP P59637
A	0	GLU	-	expression tag	UNP P59637
A	1	ASN	-	expression tag	UNP P59637
A	2	LEU	-	expression tag	UNP P59637
A	3	TYR	-	expression tag	UNP P59637
A	4	PHE	-	expression tag	UNP P59637
A	5	GLN	-	expression tag	UNP P59637
A	6	SER	-	expression tag	UNP P59637
A	7	MET	-	expression tag	UNP P59637

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Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ALA	CYS	engineered mutation	UNP P59637
A	43	ALA	CYS	engineered mutation	UNP P59637
A	44	ALA	CYS	engineered mutation	UNP P59637
B	-15	MET	-	initiating methionine	UNP P59637
B	-14	HIS	-	expression tag	UNP P59637
B	-13	HIS	-	expression tag	UNP P59637
B	-12	HIS	-	expression tag	UNP P59637
B	-11	HIS	-	expression tag	UNP P59637
B	-10	HIS	-	expression tag	UNP P59637
B	-9	HIS	-	expression tag	UNP P59637
B	-8	SER	-	expression tag	UNP P59637
B	-7	SER	-	expression tag	UNP P59637
B	-6	GLY	-	expression tag	UNP P59637
B	-5	VAL	-	expression tag	UNP P59637
B	-4	ASP	-	expression tag	UNP P59637
B	-3	LEU	-	expression tag	UNP P59637
B	-2	GLY	-	expression tag	UNP P59637
B	-1	THR	-	expression tag	UNP P59637
B	0	GLU	-	expression tag	UNP P59637
B	1	ASN	-	expression tag	UNP P59637
B	2	LEU	-	expression tag	UNP P59637
B	3	TYR	-	expression tag	UNP P59637
B	4	PHE	-	expression tag	UNP P59637
B	5	GLN	-	expression tag	UNP P59637
B	6	SER	-	expression tag	UNP P59637
B	7	MET	-	expression tag	UNP P59637
B	40	ALA	CYS	engineered mutation	UNP P59637
B	43	ALA	CYS	engineered mutation	UNP P59637
B	44	ALA	CYS	engineered mutation	UNP P59637
C	-15	MET	-	initiating methionine	UNP P59637
C	-14	HIS	-	expression tag	UNP P59637
C	-13	HIS	-	expression tag	UNP P59637
C	-12	HIS	-	expression tag	UNP P59637
C	-11	HIS	-	expression tag	UNP P59637
C	-10	HIS	-	expression tag	UNP P59637
C	-9	HIS	-	expression tag	UNP P59637
C	-8	SER	-	expression tag	UNP P59637
C	-7	SER	-	expression tag	UNP P59637
C	-6	GLY	-	expression tag	UNP P59637
C	-5	VAL	-	expression tag	UNP P59637
C	-4	ASP	-	expression tag	UNP P59637
C	-3	LEU	-	expression tag	UNP P59637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P59637
C	-1	THR	-	expression tag	UNP P59637
C	0	GLU	-	expression tag	UNP P59637
C	1	ASN	-	expression tag	UNP P59637
C	2	LEU	-	expression tag	UNP P59637
C	3	TYR	-	expression tag	UNP P59637
C	4	PHE	-	expression tag	UNP P59637
C	5	GLN	-	expression tag	UNP P59637
C	6	SER	-	expression tag	UNP P59637
C	7	MET	-	expression tag	UNP P59637
C	40	ALA	CYS	engineered mutation	UNP P59637
C	43	ALA	CYS	engineered mutation	UNP P59637
C	44	ALA	CYS	engineered mutation	UNP P59637
D	-15	MET	-	initiating methionine	UNP P59637
D	-14	HIS	-	expression tag	UNP P59637
D	-13	HIS	-	expression tag	UNP P59637
D	-12	HIS	-	expression tag	UNP P59637
D	-11	HIS	-	expression tag	UNP P59637
D	-10	HIS	-	expression tag	UNP P59637
D	-9	HIS	-	expression tag	UNP P59637
D	-8	SER	-	expression tag	UNP P59637
D	-7	SER	-	expression tag	UNP P59637
D	-6	GLY	-	expression tag	UNP P59637
D	-5	VAL	-	expression tag	UNP P59637
D	-4	ASP	-	expression tag	UNP P59637
D	-3	LEU	-	expression tag	UNP P59637
D	-2	GLY	-	expression tag	UNP P59637
D	-1	THR	-	expression tag	UNP P59637
D	0	GLU	-	expression tag	UNP P59637
D	1	ASN	-	expression tag	UNP P59637
D	2	LEU	-	expression tag	UNP P59637
D	3	TYR	-	expression tag	UNP P59637
D	4	PHE	-	expression tag	UNP P59637
D	5	GLN	-	expression tag	UNP P59637
D	6	SER	-	expression tag	UNP P59637
D	7	MET	-	expression tag	UNP P59637
D	40	ALA	CYS	engineered mutation	UNP P59637
D	43	ALA	CYS	engineered mutation	UNP P59637
D	44	ALA	CYS	engineered mutation	UNP P59637
E	-15	MET	-	initiating methionine	UNP P59637
E	-14	HIS	-	expression tag	UNP P59637
E	-13	HIS	-	expression tag	UNP P59637

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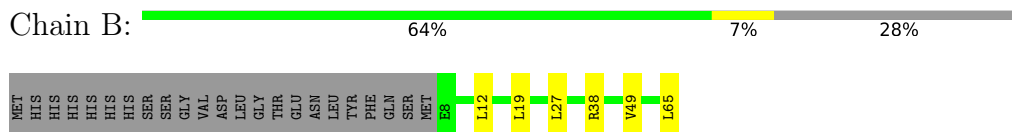| Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP P59637
E	-11	HIS	-	expression tag	UNP P59637
E	-10	HIS	-	expression tag	UNP P59637
E	-9	HIS	-	expression tag	UNP P59637
E	-8	SER	-	expression tag	UNP P59637
E	-7	SER	-	expression tag	UNP P59637
E	-6	GLY	-	expression tag	UNP P59637
E	-5	VAL	-	expression tag	UNP P59637
E	-4	ASP	-	expression tag	UNP P59637
E	-3	LEU	-	expression tag	UNP P59637
E	-2	GLY	-	expression tag	UNP P59637
E	-1	THR	-	expression tag	UNP P59637
E	0	GLU	-	expression tag	UNP P59637
E	1	ASN	-	expression tag	UNP P59637
E	2	LEU	-	expression tag	UNP P59637
E	3	TYR	-	expression tag	UNP P59637
E	4	PHE	-	expression tag	UNP P59637
E	5	GLN	-	expression tag	UNP P59637
E	6	SER	-	expression tag	UNP P59637
E	7	MET	-	expression tag	UNP P59637
E	40	ALA	CYS	engineered mutation	UNP P59637
E	43	ALA	CYS	engineered mutation	UNP P59637
E	44	ALA	CYS	engineered mutation	UNP P59637

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Envelope small membrane protein

Chain A: 62%   10%   28%

MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F20 L21 A22 F23 L27 R38 V49 L65

- Molecule 1: Envelope small membrane protein

Chain B: 64%   7%   28%

MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 L27 R38 V49 L65

- Molecule 1: Envelope small membrane protein

Chain C: 60%   11%   28%

MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F26 L27 R38 V49 K53 L65

- Molecule 1: Envelope small membrane protein

Chain D: 63%   9%   28%

MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L19 F20 L21 F26 L27 R38 V49 L65

- Molecule 1: Envelope small membrane protein

Chain E: 60%   11%   28%

MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F20 L21 A22 F23 F26 L27 R38 V49 L65

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

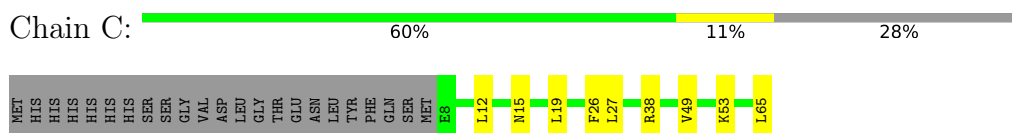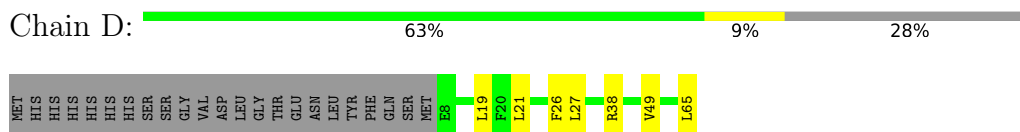### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Envelope small membrane protein

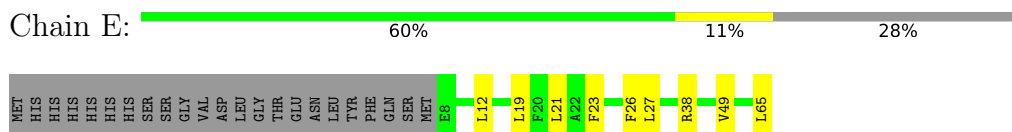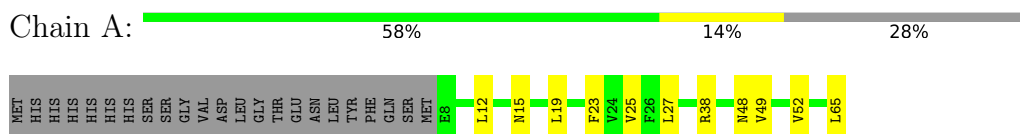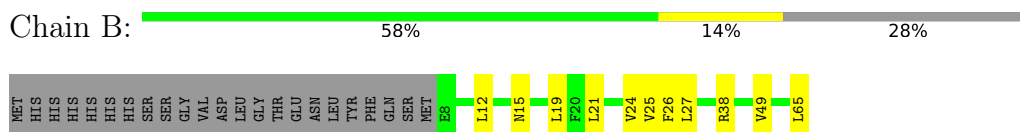
- Molecule 1: Envelope small membrane protein

- Molecule 1: Envelope small membrane protein

- Molecule 1: Envelope small membrane protein

- Molecule 1: Envelope small membrane protein

4.2.2 Score per residue for model 2

- Molecule 1: Envelope small membrane protein

- Molecule 1: Envelope small membrane protein

Chain B:

- Molecule 1: Envelope small membrane protein

Chain C:

- Molecule 1: Envelope small membrane protein

Chain D:

- Molecule 1: Envelope small membrane protein

Chain E:

4.2.3　Score per residue for model 3
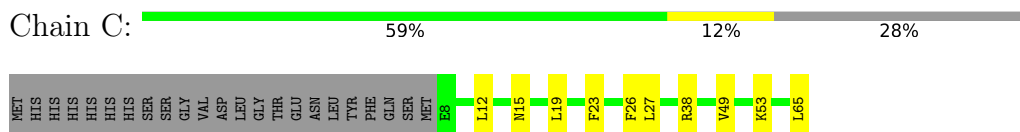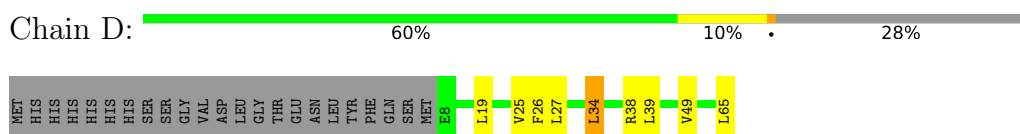
- Molecule 1: Envelope small membrane protein
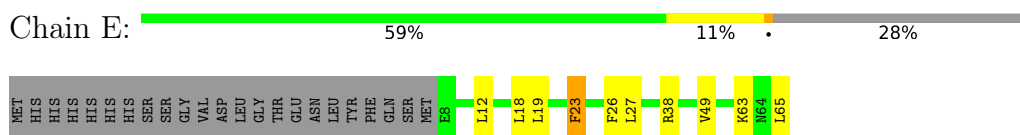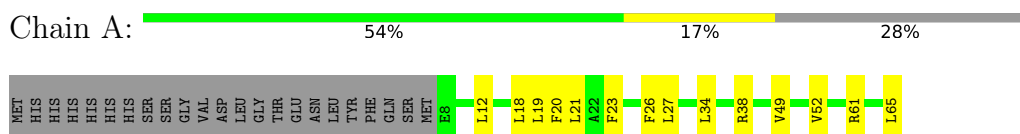
Chain A:

- Molecule 1: Envelope small membrane protein

Chain B:

- Molecule 1: Envelope small membrane protein

Chain C:

• Molecule 1: Envelope small membrane protein

Chain D:

59%   12%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F23 V24 V25 F26 L27 V49 K53 L65

• Molecule 1: Envelope small membrane protein

Chain E:

63%   7% •   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F23 V24 V25 F26 L27 V49 L65

4.2.4 Score per residue for model 4

• Molecule 1: Envelope small membrane protein

Chain A:

60%   11%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F20 L21 F26 L27 R38 V49 L65

• Molecule 1: Envelope small membrane protein

Chain B:

58%   14%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F20 L21 F26 L27 R38 L39 V49 K53 L65

• Molecule 1: Envelope small membrane protein

Chain C:

57%   15%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 S16 L19 F26 L27 T30 R38 L39 V49 R61 L65

• Molecule 1: Envelope small membrane protein

Chain D:

56%   15%   •   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F20 L21 F26 L27 L34 R38 V49 V52 Y57 R61 L65

• Molecule 1: Envelope small membrane protein

Chain E:

63%   9%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 N15 L19 F26 L27 R38 V49 L65
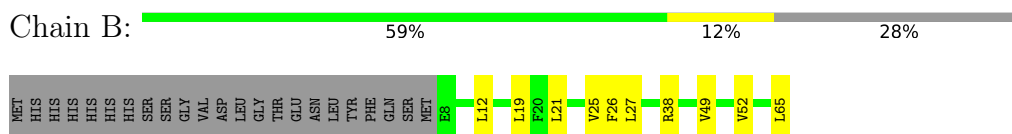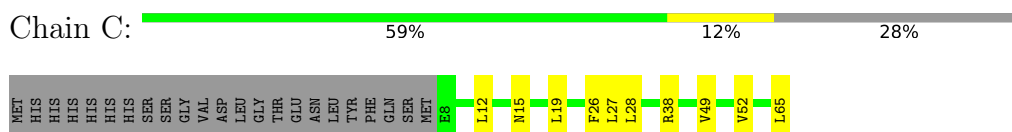
4.2.5 Score per residue for model 5

• Molecule 1: Envelope small membrane protein

Chain A:

• Molecule 1: Envelope small membrane protein

Chain B:

• Molecule 1: Envelope small membrane protein

Chain C:

• Molecule 1: Envelope small membrane protein

Chain D:

• Molecule 1: Envelope small membrane protein

Chain E:
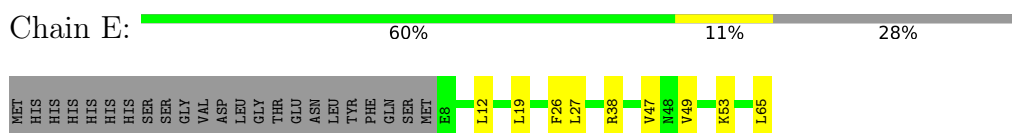
4.2.6 Score per residue for model 6
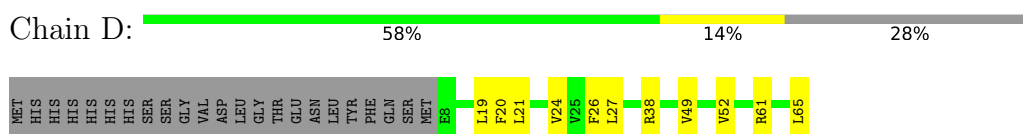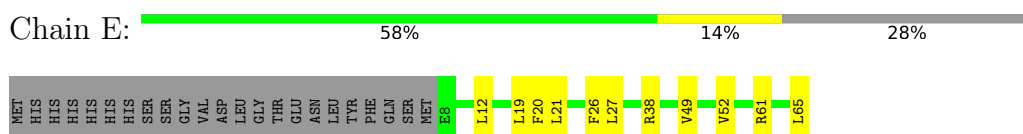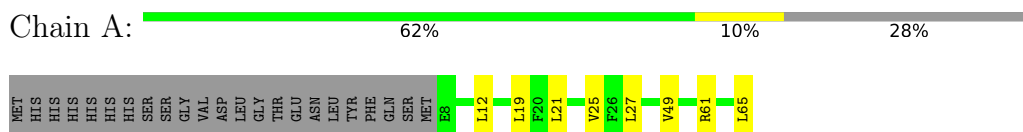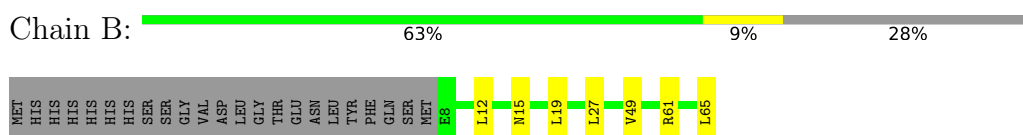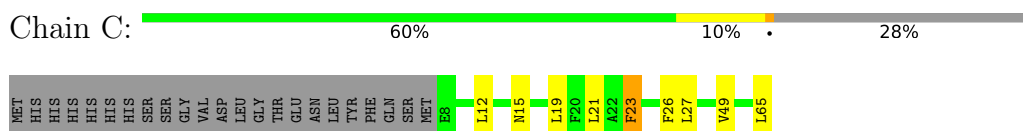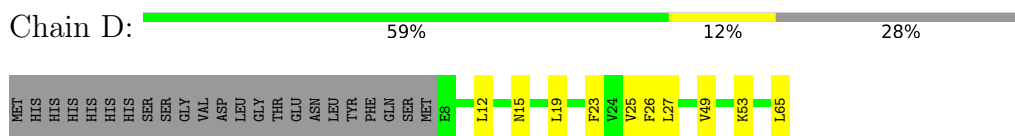
• Molecule 1: Envelope small membrane protein
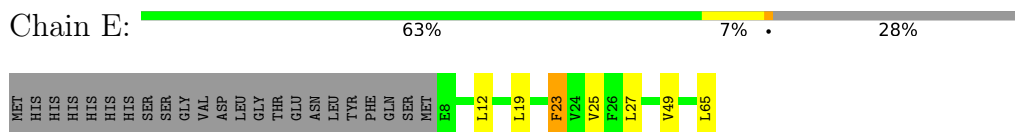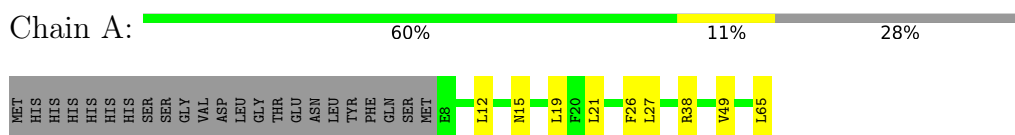
Chain A:

• Molecule 1: Envelope small membrane protein

Chain B:

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L19 F20 L21 A22 F23 L27 L34 V49 L65

- Molecule 1: Envelope small membrane protein

Chain C: 63%   9%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 L27 L34 V49 K53 L65

- Molecule 1: Envelope small membrane protein

Chain D: 63%   7%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L19 F20 L21 V24 L27 V49 V52 L65

- Molecule 1: Envelope small membrane protein

Chain E: 64%   7%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L19 F20 L21 A22 F23 V49 S50 L65

4.2.7   Score per residue for model 7

- Molecule 1: Envelope small membrane protein

Chain A: 56%   16%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L18 L19 F20 L21 A22 F23 V24 L27 R38 N45 V49 S50 L65

- Molecule 1: Envelope small membrane protein

Chain B: 62%   10%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 I13 L19 F23 L27 R38 V49 K53 L65

- Molecule 1: Envelope small membrane protein

Chain C: 64%   7%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L19 L27 R38 V49 K53 L65

- Molecule 1: Envelope small membrane protein

Chain D: 63%   9%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 I13 V14 F20 L27 L38 R38 V49 L65

• Molecule 1: Envelope small membrane protein

Chain E: 63%   7% ·   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F20 L27 R38 V49 L65

4.2.8   Score per residue for model 8

• Molecule 1: Envelope small membrane protein

Chain A: 60%   11%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F23 L27 L34 R38 V49 V52 L65

• Molecule 1: Envelope small membrane protein

Chain B: 56%   16%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 I13 V14 L19 F20 L21 A22 F23 L27 L34 R38 V49 V52 K53 Y57 L65

• Molecule 1: Envelope small membrane protein

Chain C: 58%   12% ·   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 L27 L34 R38 V49 V52 K53 P54 T55 V58 L65

• Molecule 1: Envelope small membrane protein

Chain D: 54%   17%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L18 L19 F20 L21 V24 L27 R38 V47 N48 V49 V52 Y57 V58 V62 L65

• Molecule 1: Envelope small membrane protein

Chain E: 58%   14%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F23 F26 L27 R38 V49 T55 V58 V62 L65
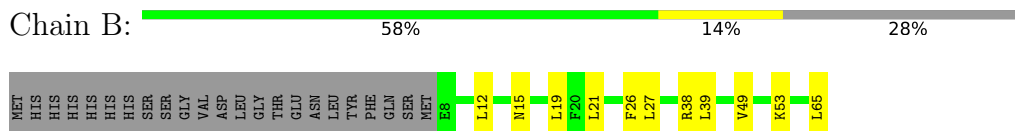
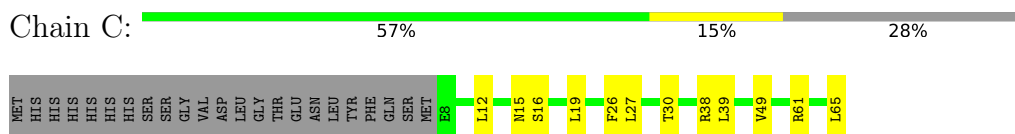### 4.2.9 Score per residue for model 9

• Molecule 1: Envelope small membrane protein

Chain A:

• Molecule 1: Envelope small membrane protein

Chain B:

• Molecule 1: Envelope small membrane protein

Chain C:

• Molecule 1: Envelope small membrane protein

Chain D:

• Molecule 1: Envelope small membrane protein

Chain E:

4.2.10 Score per residue for model 10
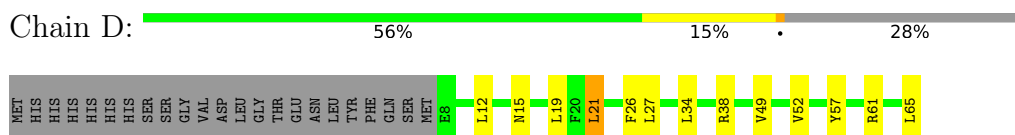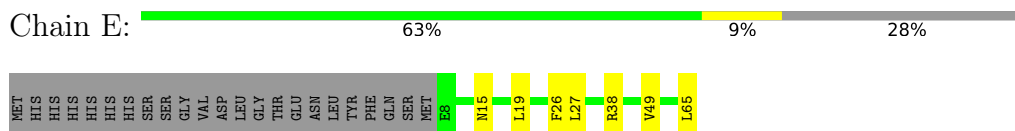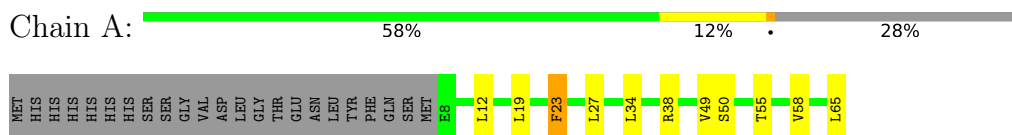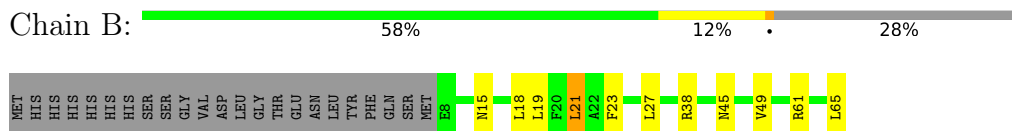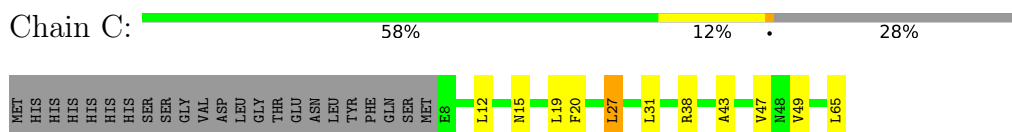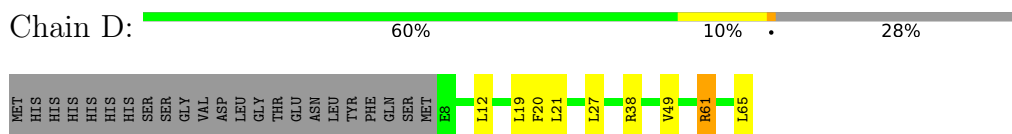
• Molecule 1: Envelope small membrane protein
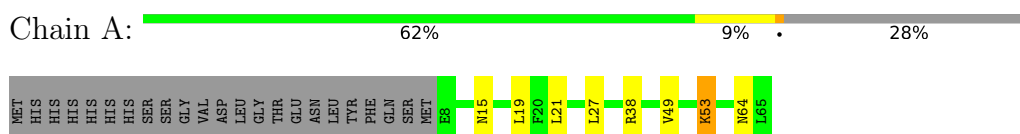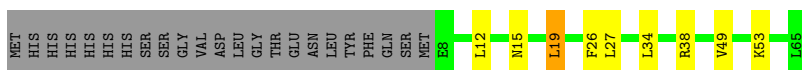
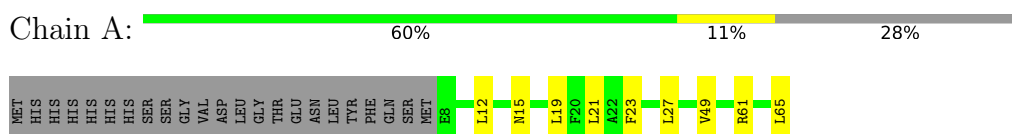Chain A:

• Molecule 1: Envelope small membrane protein

Chain B:

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F26 L27 L34 R38 V49 K53 L65

• Molecule 1: Envelope small membrane protein

Chain C: 59% 12% 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 N15 L18 L19 F20 L21 V25 F26 L27 R38 V49 K53 L65

• Molecule 1: Envelope small membrane protein

Chain D: 60% 10% · 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F20 L21 F26 L27 R38 V49 K53 N64 L65

• Molecule 1: Envelope small membrane protein

Chain E: 59% 12% 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F20 L21 F26 L27 R38 V49 K53 N64 L65
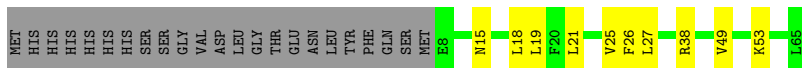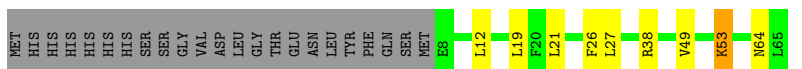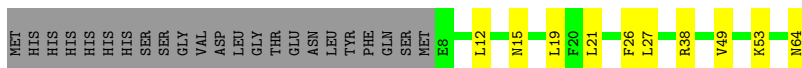
4.2.11   Score per residue for model 11

• Molecule 1: Envelope small membrane protein
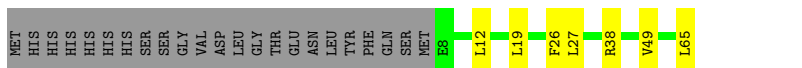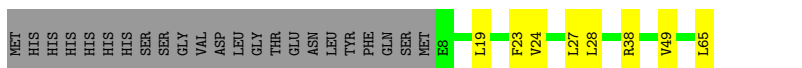
Chain A: 63% 9% 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F26 L27 R38 V49 L65

• Molecule 1: Envelope small membrane protein

Chain B: 62% 10% 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L19 F23 V24 L27 L28 R38 V49 L65

• Molecule 1: Envelope small membrane protein

Chain C: 64% 7% 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L19 L27 R38 V49 K53 N64 L65

• Molecule 1: Envelope small membrane protein

Chain D: 57% 14% · 28%

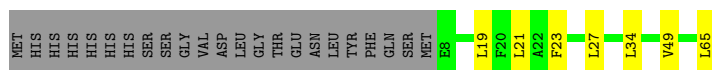• Molecule 1: Envelope small membrane protein

Chain E:
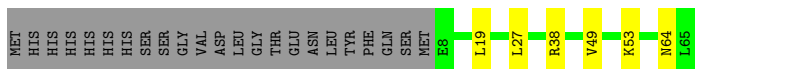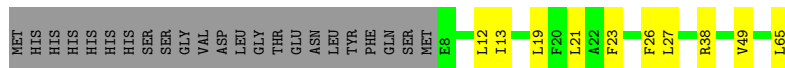
4.2.12 Score per residue for model 12
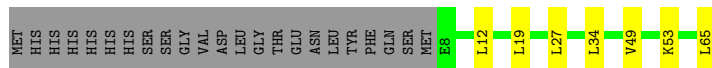
• Molecule 1: Envelope small membrane protein
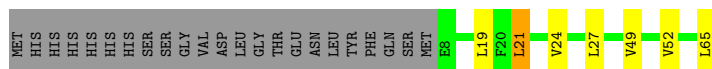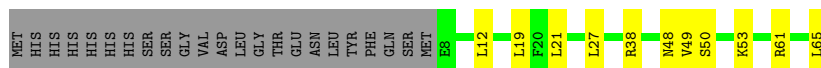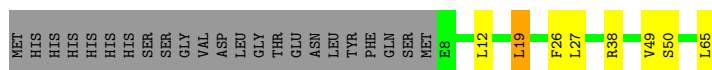
Chain A:

• Molecule 1: Envelope small membrane protein

Chain B:

• Molecule 1: Envelope small membrane protein

Chain C:

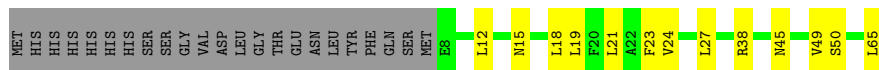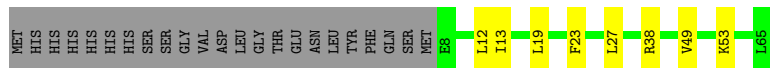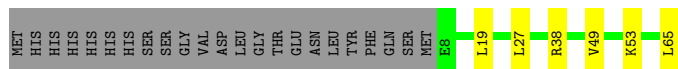

• Molecule 1: Envelope small membrane protein

Chain D:

• Molecule 1: Envelope small membrane protein

Chain E:
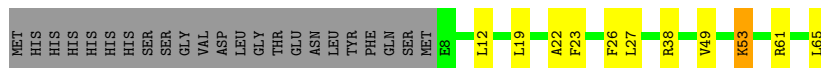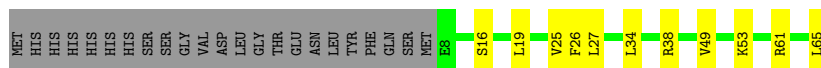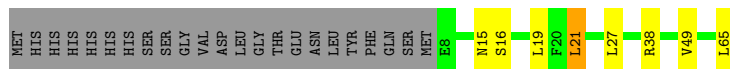
4.2.13 Score per residue for model 13

• Molecule 1: Envelope small membrane protein
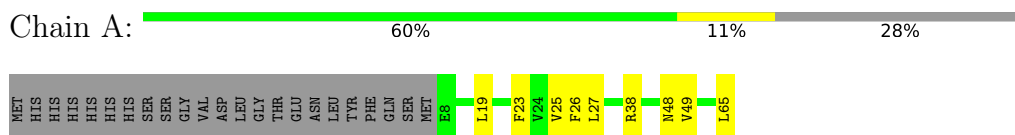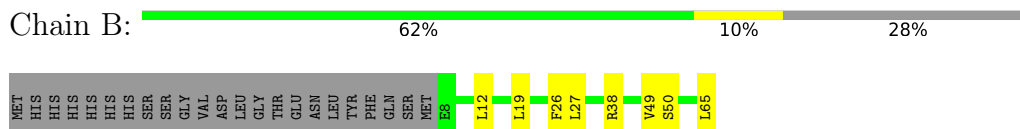
Chain A:

Chain A: 60% 11% 28%

• Molecule 1: Envelope small membrane protein

Chain B: 62% 10% 28%

• Molecule 1: Envelope small membrane protein

Chain C: 62% 10% 28%

• Molecule 1: Envelope small membrane protein

Chain D: 54% 17% 28%

• Molecule 1: Envelope small membrane protein

Chain E: 57% 12% 28%
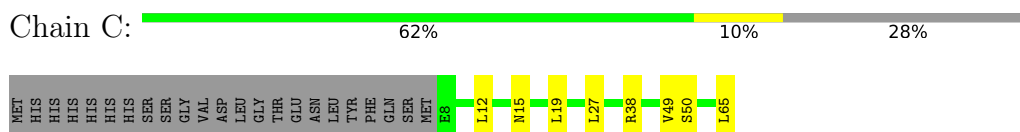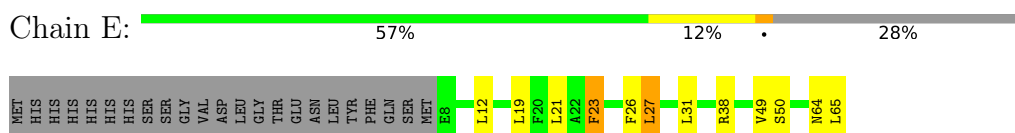
4.2.14 Score per residue for model 14

• Molecule 1: Envelope small membrane protein

Chain A: 59% 11% 28%

• Molecule 1: Envelope small membrane protein

Chain B: 57% 15% 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F23 F26 L27 R38 A43 V47 M48 V49 K53 R61 L65

- Molecule 1: Envelope small membrane protein

Chain C: 58%   14%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 L19 F23 F26 L27 R38 V49 K53 P54 T55 V58 R61 L65

- Molecule 1: Envelope small membrane protein

Chain D: 59%   12%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 T11 L19 F26 L27 R38 V49 K53 R61 L65

- Molecule 1: Envelope small membrane protein

Chain E: 57%   14% · 28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 I13 V14 N15 S16 V17 L18 L19 F26 L27 R38 L39 V49 K53 R61 L65

4.2.15 Score per residue for model 15

- Molecule 1: Envelope small membrane protein
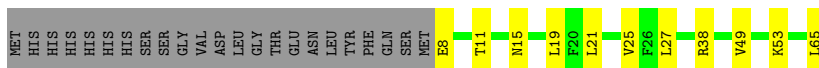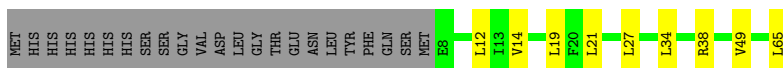
Chain A: 58%   14%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 T11 N15 L19 F20 L21 V25 F26 L27 R38 V49 K53 L65

- Molecule 1: Envelope small membrane protein

Chain B: 60%   11%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 I13 V14 L19 F20 L21 L27 L34 R38 V49 L65

- Molecule 1: Envelope small membrane protein

Chain C: 59%   12%   28%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET E8 L12 N15 L19 F26 L27 L34 R38 V49 R61 L65

- Molecule 1: Envelope small membrane protein

Chain D: 60%   11%   28%

• Molecule 1: Envelope small membrane protein

Chain E:
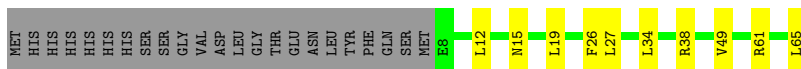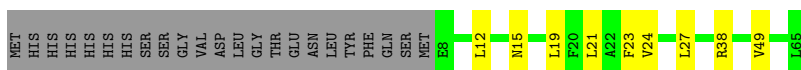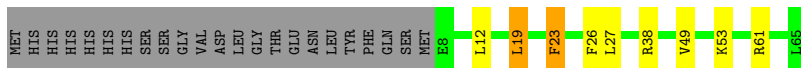
4.2.16 Score per residue for model 16

• Molecule 1: Envelope small membrane protein
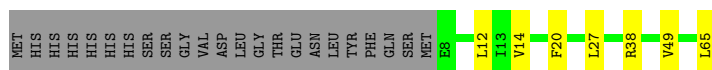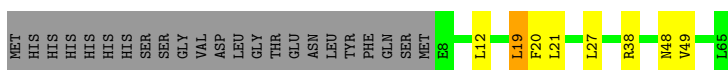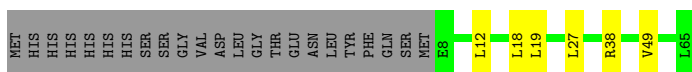
Chain A:

• Molecule 1: Envelope small membrane protein

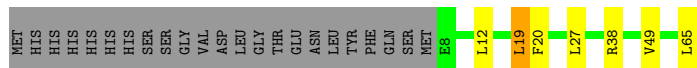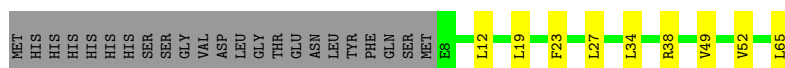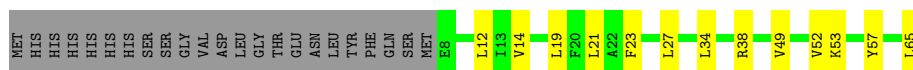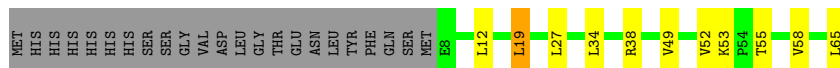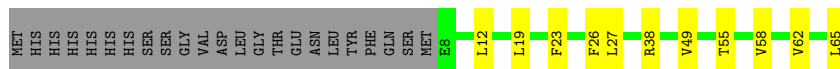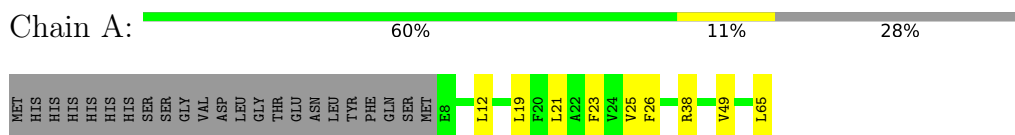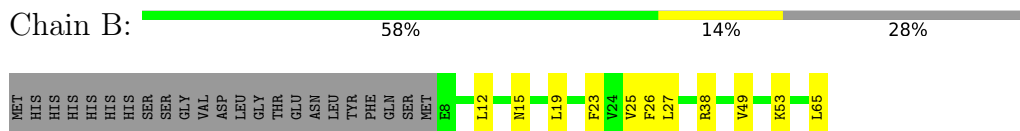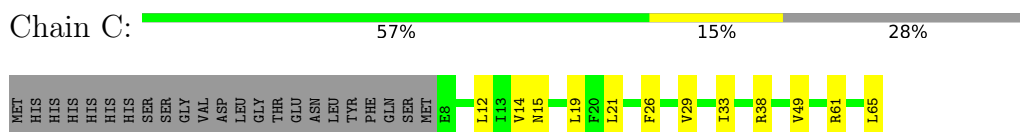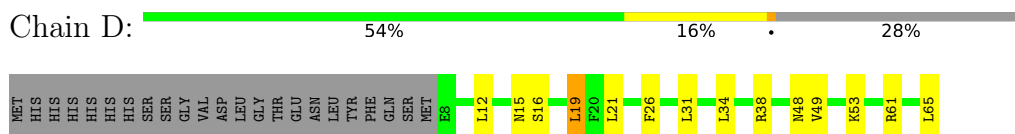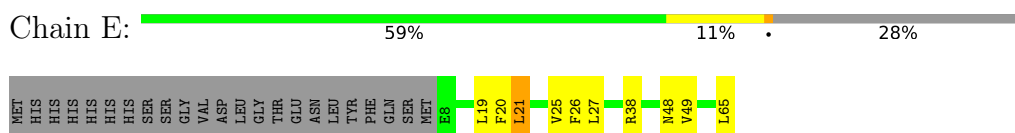Chain B:

• Molecule 1: Envelope small membrane protein

Chain C:

• Molecule 1: Envelope small membrane protein

Chain D:

• Molecule 1: Envelope small membrane protein

Chain E:
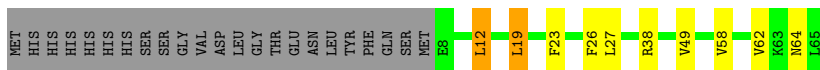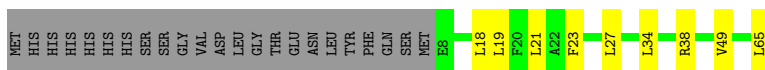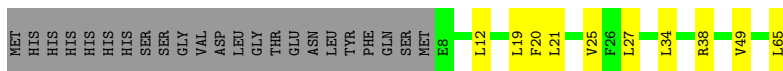
5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing.*

Of the 200 calculated structures, 16 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.0
HADDOCK	refinement	2.2

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	811
Number of shifts mapped to atoms	811
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	19%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	447	495	494	2±2
1	B	447	495	494	1±1
1	C	447	495	494	1±1
1	D	447	495	494	2±1
1	E	447	495	494	2±1
All	All	35760	39600	39520	74

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:25:VAL:HB	1:E:23:PHE:CZ	0.67	2.25	1	2
1:C:23:PHE:CZ	1:D:21:LEU:HD13	0.64	2.28	16	1
1:A:55:THR:O	1:A:58:VAL:HG22	0.60	1.96	5	1
1:A:18:LEU:O	1:E:19:LEU:HG	0.60	1.97	7	1
1:D:23:PHE:CZ	1:E:25:VAL:HG21	0.56	2.35	3	1
1:B:19:LEU:HD12	1:C:25:VAL:HG21	0.56	1.76	10	1
1:C:23:PHE:CZ	1:D:25:VAL:HG11	0.56	2.36	12	1
1:D:23:PHE:CZ	1:E:25:VAL:HB	0.56	2.35	16	1
1:D:16:SER:HA	1:E:21:LEU:HD21	0.55	1.78	11	3
1:B:15:ASN:OD1	1:C:18:LEU:HA	0.54	2.02	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:25:VAL:CG2	1:E:19:LEU:HG	0.54	2.32	9	1
1:D:21:LEU:O	1:D:24:VAL:HG12	0.54	2.03	6	5
1:A:19:LEU:HG	1:B:18:LEU:O	0.52	2.04	16	1
1:D:23:PHE:CE2	1:E:25:VAL:HG21	0.51	2.41	3	1
1:A:21:LEU:HG	1:E:19:LEU:HD23	0.51	1.82	15	1
1:C:23:PHE:CE2	1:D:25:VAL:HG21	0.50	2.41	1	1
1:C:19:LEU:HD21	1:D:18:LEU:HB3	0.50	1.84	16	1
1:D:23:PHE:CE2	1:E:25:VAL:HB	0.50	2.41	16	1
1:D:27:LEU:O	1:D:31:LEU:HG	0.50	2.05	11	1
1:C:23:PHE:CZ	1:D:25:VAL:HB	0.48	2.43	3	1
1:A:25:VAL:HB	1:E:23:PHE:CE2	0.48	2.44	1	2
1:A:25:VAL:HG12	1:E:23:PHE:CD2	0.47	2.44	15	1
1:B:19:LEU:HD11	1:C:22:ALA:HA	0.47	1.86	12	1
1:A:25:VAL:HG21	1:E:19:LEU:HD12	0.47	1.86	14	1
1:C:19:LEU:HG	1:D:18:LEU:O	0.46	2.11	8	1
1:D:8:GLU:HA	1:D:11:THR:OG1	0.46	2.11	14	1
1:A:21:LEU:CD2	1:E:16:SER:HA	0.46	2.41	14	1
1:A:25:VAL:HG21	1:E:19:LEU:CD1	0.45	2.42	14	1
1:A:21:LEU:O	1:A:24:VAL:HG12	0.45	2.10	14	2
1:C:12:LEU:HG	1:C:12:LEU:O	0.45	2.10	16	1
1:C:27:LEU:HA	1:C:30:THR:HG22	0.45	1.89	4	1
1:D:31:LEU:HD23	1:D:34:LEU:HD21	0.45	1.89	9	1
1:A:23:PHE:CE2	1:B:25:VAL:HG21	0.45	2.47	1	1
1:C:16:SER:HA	1:D:21:LEU:HD21	0.45	1.88	4	1
1:C:27:LEU:O	1:C:31:LEU:HB2	0.44	2.13	5	1
1:D:58:VAL:O	1:D:62:VAL:HG23	0.44	2.12	8	1
1:E:27:LEU:O	1:E:31:LEU:HB2	0.44	2.13	13	1
1:C:23:PHE:CE1	1:D:25:VAL:HG11	0.44	2.47	1	1
1:D:61:ARG:NH2	1:E:47:VAL:HG13	0.43	2.27	5	1
1:C:58:VAL:O	1:C:62:VAL:HG23	0.43	2.14	16	1
1:E:58:VAL:O	1:E:62:VAL:HG23	0.43	2.14	8	1
1:A:8:GLU:HA	1:A:11:THR:OG1	0.43	2.14	15	1
1:C:23:PHE:HZ	1:D:25:VAL:HG11	0.42	1.72	12	1
1:A:23:PHE:CD2	1:B:21:LEU:HD13	0.42	2.50	5	1
1:A:48:ASN:HA	1:E:63:LYS:NZ	0.42	2.30	1	1
1:A:23:PHE:CE2	1:B:21:LEU:HD13	0.42	2.50	5	1
1:C:55:THR:O	1:C:58:VAL:HG22	0.42	2.15	8	2
1:E:13:ILE:O	1:E:17:VAL:HG23	0.42	2.15	14	1
1:A:45:ASN:O	1:A:50:SER:HB2	0.41	2.14	7	1
1:C:19:LEU:HD21	1:D:18:LEU:CB	0.41	2.44	16	1
1:A:21:LEU:HD22	1:E:19:LEU:HB3	0.41	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:C:43:ALA:O	1:C:47:VAL:HG23	0.41	2.14	5	1
1:E:55:THR:O	1:E:58:VAL:HG22	0.41	2.16	8	1
1:A:21:LEU:HD21	1:E:16:SER:HA	0.41	1.93	12	1
1:B:21:LEU:O	1:B:24:VAL:HG12	0.41	2.15	1	1
1:B:21:LEU:O	1:B:25:VAL:HG22	0.41	2.16	2	1
1:A:21:LEU:HD22	1:E:16:SER:HA	0.41	1.91	14	1
1:A:48:ASN:HA	1:E:64:ASN:OD1	0.41	2.16	13	1
1:C:29:VAL:O	1:C:33:ILE:HG13	0.40	2.16	9	1
1:D:19:LEU:HD12	1:E:25:VAL:HG21	0.40	1.92	9	1
1:C:23:PHE:CZ	1:D:25:VAL:HG21	0.40	2.50	12	1
1:D:34:LEU:O	1:D:39:LEU:HG	0.40	2.16	1	1
1:B:43:ALA:O	1:B:47:VAL:HG23	0.40	2.17	14	1
1:A:23:PHE:CE2	1:B:25:VAL:HB	0.40	2.52	9	1

6.3   Torsion angles ⓘ

6.3.1   Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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	A	56/81 (69%)	50±1 (89±2%)	5±1 (9±2%)	1±0 (2±1%)	10	49
1	B	56/81 (69%)	49±2 (87±3%)	6±2 (10±3%)	1±1 (2±1%)	9	45
1	C	56/81 (69%)	50±1 (88±2%)	5±1 (9±2%)	1±0 (3±1%)	8	44
1	D	56/81 (69%)	50±1 (89±2%)	5±1 (9±3%)	1±0 (2±1%)	9	45
1	E	56/81 (69%)	49±1 (88±2%)	6±1 (10±3%)	1±0 (2±1%)	9	48
All	All	4480/6480 (69%)	3949 (88%)	423 (9%)	108 (2%)	9	46

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	49	VAL	16
1	B	49	VAL	16
1	C	49	VAL	16
1	D	49	VAL	16

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Mol	Chain	Res	Type	Models (Total)
1	E	49	VAL	16
1	C	53	LYS	6
1	D	53	LYS	6
1	B	53	LYS	4
1	E	53	LYS	4
1	A	53	LYS	4
1	B	39	LEU	1
1	C	39	LEU	1
1	B	13	ILE	1
1	E	13	ILE	1

6.3.2   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 NMR 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	A	50/71 (70%)	43±2 (86±4%)	7±2 (14±4%)	6	45
1	B	50/71 (70%)	43±2 (85±4%)	7±2 (15±4%)	6	45
1	C	50/71 (70%)	43±2 (86±3%)	7±2 (14±3%)	6	46
1	D	50/71 (70%)	43±2 (85±4%)	7±2 (15±4%)	6	44
1	E	50/71 (70%)	43±1 (86±3%)	7±1 (14±3%)	6	46
All	All	4000/5680 (70%)	3424 (86%)	576 (14%)	6	45

All 96 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	19	LEU	16
1	B	19	LEU	16
1	B	27	LEU	16
1	C	19	LEU	16
1	A	27	LEU	15
1	D	19	LEU	15
1	D	27	LEU	15
1	E	19	LEU	15
1	E	27	LEU	15
1	A	38	ARG	14

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Mol	Chain	Res	Type	Models (Total)
1	B	38	ARG	14
1	C	27	LEU	14
1	C	38	ARG	14
1	D	38	ARG	14
1	D	65	LEU	14
1	E	38	ARG	14
1	A	65	LEU	13
1	B	12	LEU	13
1	C	12	LEU	13
1	E	65	LEU	13
1	A	12	LEU	12
1	B	65	LEU	12
1	C	65	LEU	12
1	E	12	LEU	11
1	E	26	PHE	11
1	C	26	PHE	10
1	D	26	PHE	10
1	C	15	ASN	9
1	B	26	PHE	8
1	A	21	LEU	8
1	D	12	LEU	8
1	A	15	ASN	7
1	E	23	PHE	7
1	E	21	LEU	7
1	B	23	PHE	7
1	B	15	ASN	6
1	A	23	PHE	6
1	A	26	PHE	6
1	D	61	ARG	6
1	D	34	LEU	5
1	D	15	ASN	5
1	B	21	LEU	5
1	C	61	ARG	5
1	D	21	LEU	5
1	A	61	ARG	4
1	D	20	PHE	4
1	D	52	VAL	4
1	E	20	PHE	4
1	E	15	ASN	4
1	B	34	LEU	4
1	A	52	VAL	3
1	A	34	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	E	61	ARG	3
1	B	61	ARG	3
1	C	21	LEU	3
1	C	34	LEU	3
1	C	53	LYS	3
1	A	20	PHE	2
1	B	52	VAL	2
1	C	52	VAL	2
1	C	23	PHE	2
1	D	57	TYR	2
1	A	50	SER	2
1	E	50	SER	2
1	B	14	VAL	2
1	B	53	LYS	2
1	D	47	VAL	2
1	D	48	ASN	2
1	C	64	ASN	2
1	A	48	ASN	2
1	B	50	SER	2
1	D	23	PHE	2
1	E	18	LEU	1
1	A	18	LEU	1
1	C	28	LEU	1
1	E	52	VAL	1
1	B	18	LEU	1
1	B	45	ASN	1
1	C	20	PHE	1
1	D	14	VAL	1
1	B	57	TYR	1
1	C	14	VAL	1
1	E	48	ASN	1
1	A	53	LYS	1
1	A	64	ASN	1
1	D	53	LYS	1
1	D	64	ASN	1
1	E	64	ASN	1
1	B	24	VAL	1
1	B	28	LEU	1
1	C	50	SER	1
1	D	25	VAL	1
1	D	28	LEU	1
1	D	50	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	E	39	LEU	1
1	E	34	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 19% for the well-defined parts and 19% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *7_BMRB_Etr.txt*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	811
Number of shifts mapped to atoms	811
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	58	-0.82 ± 0.21	Should be checked
$^{13}C_\beta$	57	0.18 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	52	2.91 ± 0.17	Should be applied
^{15}N	57	0.70 ± 0.25	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 19%, i.e. 811 atoms were assigned a chemical shift out of a possible 4210. 0 out of 115 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	283/1445 (20%)	116/580 (20%)	110/580 (19%)	57/285 (20%)
Sidechain	482/2480 (19%)	332/1675 (20%)	142/745 (19%)	8/60 (13%)

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	46/285 (16%)	24/135 (18%)	22/150 (15%)	0/0 (—%)
Overall	811/4210 (19%)	472/2390 (20%)	274/1475 (19%)	65/345 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 811 atoms were assigned a chemical shift out of a possible 4210. 0 out of 115 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	283/1445 (20%)	116/580 (20%)	110/580 (19%)	57/285 (20%)
Sidechain	482/2480 (19%)	332/1675 (20%)	142/745 (19%)	8/60 (13%)
Aromatic	46/285 (16%)	24/135 (18%)	22/150 (15%)	0/0 (—%)
Overall	811/4210 (19%)	472/2390 (20%)	274/1475 (19%)	65/345 (19%)

7.1.4   Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5   Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:
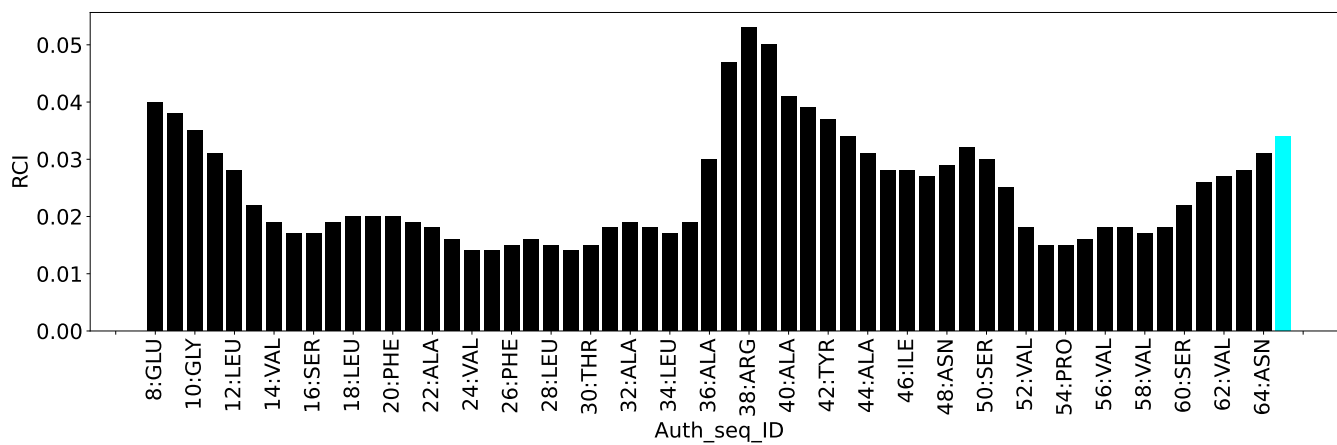
8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	556
Intra-residue ($|i-j|=0$)	208
Sequential ($|i-j|=1$)	191
Medium range ($|i-j|>1$ and $|i-j|<5$)	107
Long range ($|i-j|{\geq}5$)	0
Inter-chain	50
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	1.4
Number of long range restraints per residue[1]	0.0

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations ⓘ

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model ⓘ

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	13.9	0.2
0.2-0.5 (Medium)	24.3	0.5
>0.5 (Large)	29.8	7.05

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	208	37.4	22	10.6	4.0	3	1.4	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	199	35.8	22	11.1	4.0	3	1.5	0.5
Sidechain-Sidechain	9	1.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	191	34.4	30	15.7	5.4	9	4.7	1.6
Backbone-Backbone	53	9.5	3	5.7	0.5	0	0.0	0.0
Backbone-Sidechain	137	24.6	26	19.0	4.7	9	6.6	1.6
Sidechain-Sidechain	1	0.2	1	100.0	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	107	19.2	30	28.0	5.4	11	10.3	2.0
Backbone-Backbone	84	15.1	18	21.4	3.2	6	7.1	1.1
Backbone-Sidechain	22	4.0	11	50.0	2.0	5	22.7	0.9
Sidechain-Sidechain	1	0.2	1	100.0	0.2	0	0.0	0.0
Long range (|i-j|≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	50	9.0	36	72.0	6.5	5	10.0	0.9
Backbone-Backbone	15	2.7	15	100.0	2.7	5	33.3	0.9
Backbone-Sidechain	35	6.3	21	60.0	3.8	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	556	100.0	118	21.2	21.2	28	5.0	5.0
Backbone-Backbone	152	27.3	36	23.7	6.5	11	7.2	2.0
Backbone-Sidechain	393	70.7	80	20.4	14.4	17	4.3	3.1
Sidechain-Sidechain	11	2.0	2	18.2	0.4	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations ⓘ
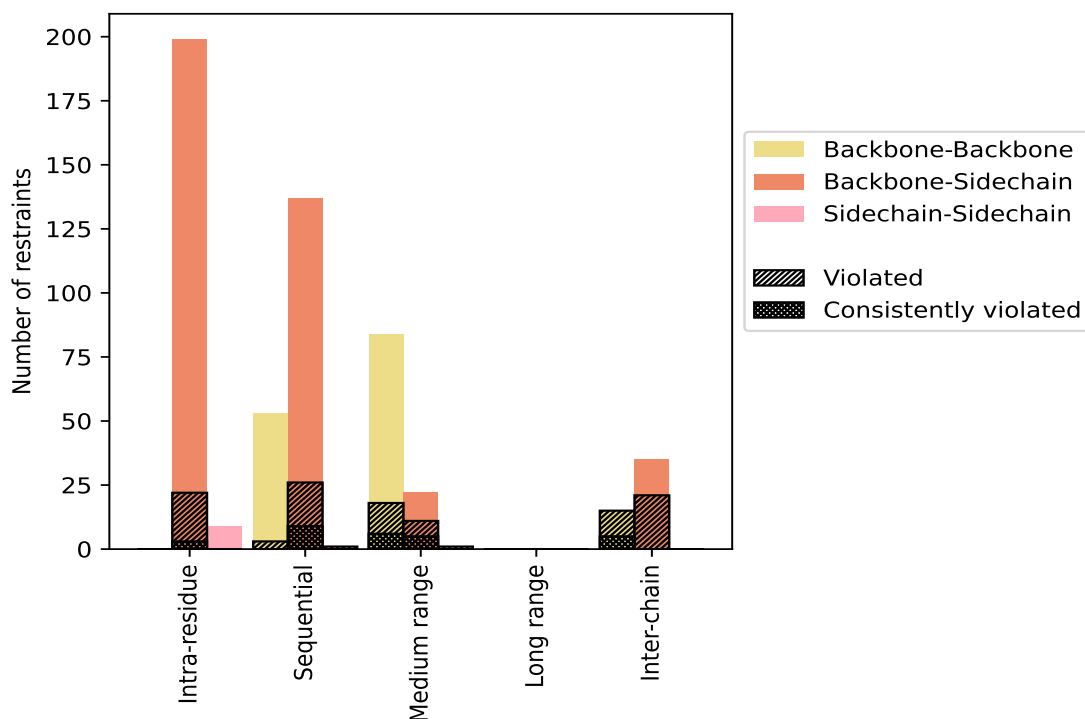
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model ⓘ

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	10	19	18	0	18	65	0.75	3.43	0.82	0.37
2	13	21	21	0	11	66	0.84	4.11	0.94	0.44
3	16	21	21	0	10	68	0.65	3.21	0.73	0.34
4	12	19	22	0	16	69	0.74	3.31	0.77	0.38
5	12	21	17	0	15	65	0.76	4.62	0.97	0.35
6	12	20	17	0	17	66	0.81	4.09	0.94	0.43
7	9	22	19	0	19	69	0.86	3.59	0.96	0.37
8	9	20	18	0	20	67	1.02	4.21	1.1	0.52
9	13	18	19	0	19	69	0.69	3.58	0.74	0.36
10	13	19	20	0	17	69	0.82	4.5	0.98	0.42
11	12	20	18	0	20	70	0.88	3.82	0.98	0.44

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	13	19	18	0	17	67	0.9	4.44	0.96	0.47
13	9	21	15	0	16	61	0.85	4.22	0.96	0.37
14	13	19	20	0	19	71	0.93	4.81	1.09	0.53
15	10	18	19	0	23	70	1.14	5.61	1.24	0.56
16	12	19	20	0	25	76	1.07	7.05	1.36	0.46

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ
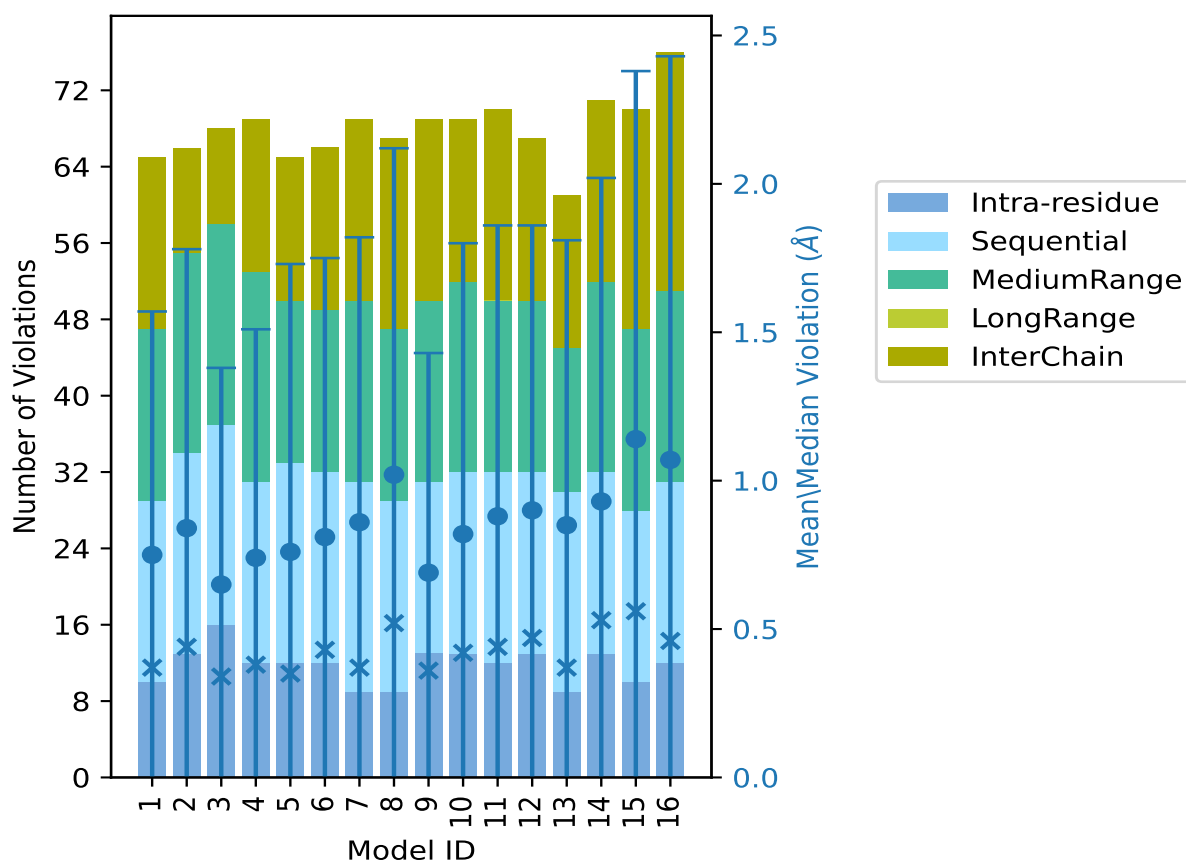
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 438(IR:186, SQ:161, MR:77, LR:0, IC:14) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
4	1	3	0	2	10	1	6.2
1	3	6	0	1	11	2	12.5
2	4	0	0	4	10	3	18.8
0	0	0	0	2	2	4	25.0
1	1	1	0	5	8	5	31.2
2	0	1	0	3	6	6	37.5
0	2	0	0	0	2	7	43.8
0	0	0	0	5	5	8	50.0
0	0	0	0	3	3	9	56.2
1	1	0	0	2	4	10	62.5
2	1	4	0	0	7	11	68.8
1	1	1	0	4	7	12	75.0
3	2	0	0	0	5	13	81.2
2	0	1	0	0	3	14	87.5
0	5	2	0	0	7	15	93.8
3	9	11	0	5	28	16	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble (i)
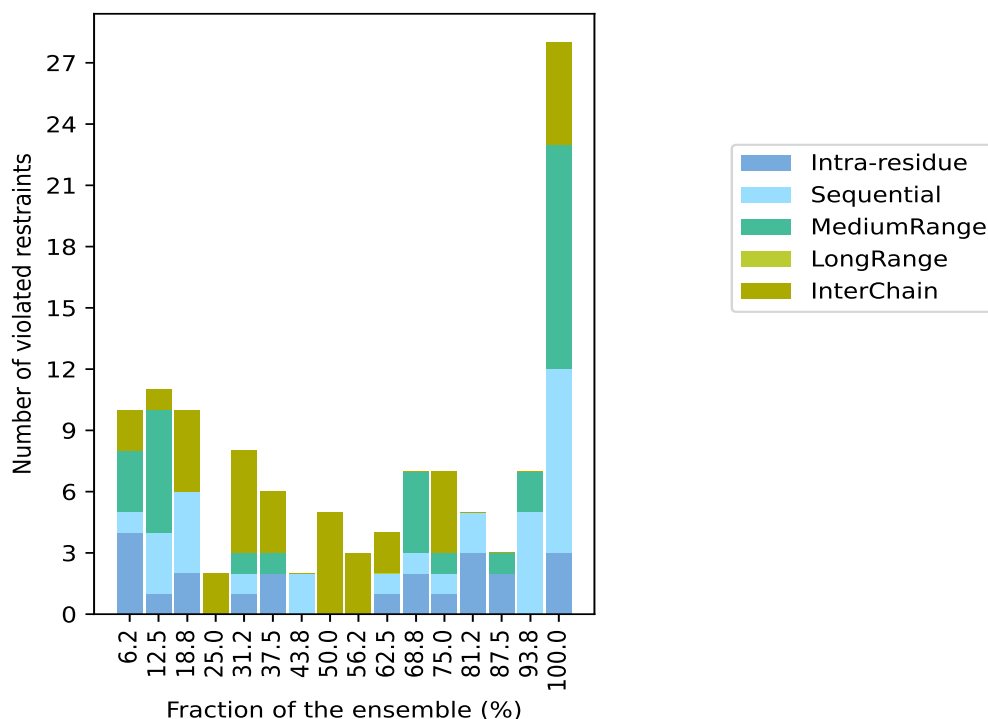
9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble
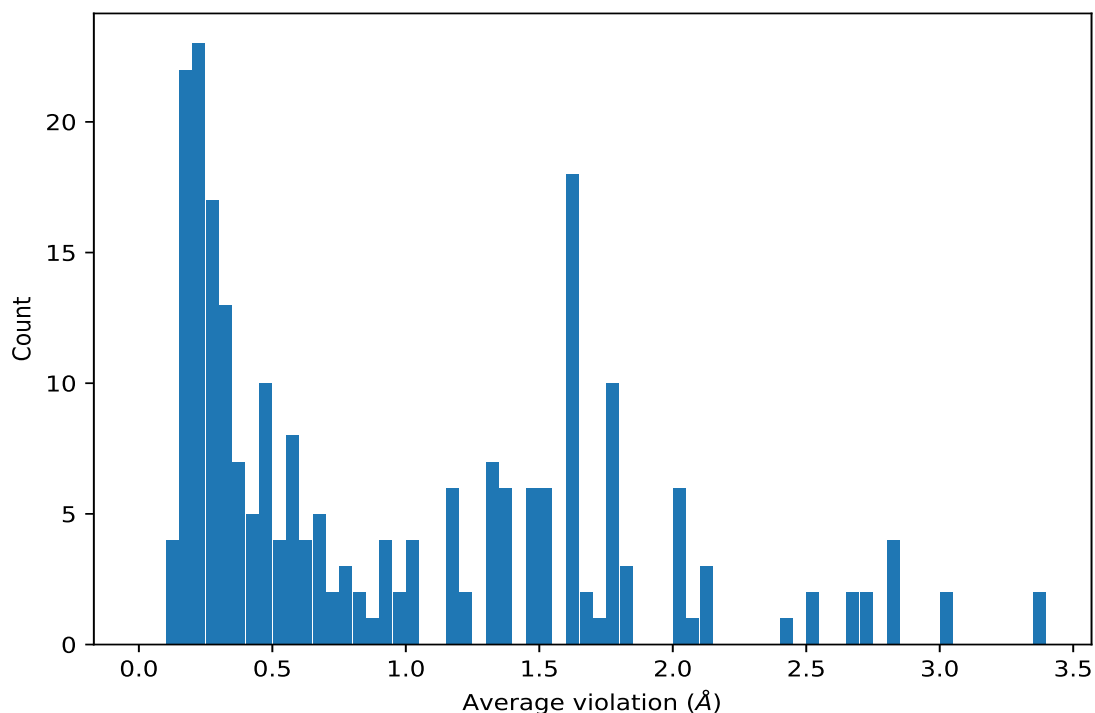
9.4.2 Table: Most violated distance restraints ⓘ

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	16	3.03	1.19	3.1
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	16	3.03	1.19	3.1
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	16	2.82	0.96	2.7
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	16	2.82	0.96	2.7
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	16	2.7	1.11	3.08
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	16	2.7	1.11	3.08
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	16	2.66	1.16	2.93
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	16	2.66	1.16	2.93
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	16	2.12	0.79	2.18
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	16	2.12	0.79	2.18
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	16	1.78	0.21	1.82
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	16	1.78	0.21	1.82
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	16	1.74	0.3	1.78
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	16	1.48	0.15	1.46
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	16	1.48	0.15	1.46
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	16	1.48	0.15	1.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	16	1.48	0.15	1.46
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	16	1.48	0.15	1.46
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	16	1.48	0.15	1.46
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	16	0.78	0.16	0.76
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	16	0.73	0.03	0.74
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	16	0.73	0.03	0.74
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	16	0.69	0.15	0.64
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	16	0.67	0.22	0.7
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	16	0.65	0.26	0.6
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	16	0.63	0.21	0.72
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	16	0.57	0.08	0.57
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	16	0.57	0.08	0.57
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	16	0.57	0.08	0.57
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	16	0.54	0.06	0.55
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	16	0.48	0.1	0.46
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	16	0.48	0.1	0.46
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	16	0.48	0.1	0.46
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	16	0.45	0.08	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	16	0.45	0.08	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	16	0.45	0.08	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	16	0.45	0.08	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	16	0.45	0.08	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	16	0.45	0.08	0.44
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	16	0.44	0.14	0.4
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	16	0.44	0.14	0.4
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	16	0.44	0.14	0.4
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	16	0.38	0.04	0.36
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	16	0.38	0.04	0.36
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	16	0.33	0.13	0.3
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	16	0.31	0.11	0.31
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	16	0.31	0.11	0.31
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	16	0.3	0.03	0.31
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	16	0.3	0.03	0.3
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	16	0.29	0.1	0.29
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	16	0.29	0.1	0.29
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	16	0.25	0.03	0.24
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	16	0.23	0.01	0.23
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	16	0.21	0.03	0.2
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	15	1.01	0.24	1.0
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	15	1.01	0.24	1.0
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	15	0.93	0.23	0.9
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	15	0.93	0.23	0.9

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	15	0.93	0.23	0.9
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	15	0.93	0.23	0.9
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	15	0.88	0.41	1.03
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	15	0.63	0.24	0.59
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	15	0.32	0.06	0.32
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	15	0.32	0.06	0.32
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	15	0.21	0.06	0.21
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	15	0.17	0.05	0.16
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	14	0.4	0.1	0.38
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	14	0.34	0.13	0.35
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	14	0.34	0.13	0.35
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	14	0.14	0.01	0.15
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	13	0.29	0.06	0.31
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	13	0.29	0.06	0.31
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	13	0.28	0.1	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	13	0.28	0.1	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	13	0.28	0.1	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	13	0.28	0.1	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	13	0.28	0.1	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	13	0.28	0.1	0.27
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	13	0.21	0.08	0.2
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	13	0.21	0.08	0.2
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	13	0.16	0.04	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	13	0.15	0.02	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	13	0.15	0.02	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	13	0.15	0.02	0.14
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	12	3.35	1.36	3.34
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	12	3.35	1.36	3.34
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	12	2.82	1.53	2.92
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	12	2.82	1.53	2.92
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	12	1.84	1.74	1.44
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	12	1.81	1.16	1.42
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	12	1.81	1.16	1.42
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	12	0.8	0.29	0.93
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	12	0.8	0.29	0.93
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	12	0.46	0.19	0.36
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	12	0.29	0.11	0.31
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	11	0.39	0.21	0.32
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	11	0.32	0.12	0.35
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	11	0.31	0.09	0.29
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	11	0.24	0.09	0.21
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	11	0.24	0.09	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	11	0.22	0.1	0.19
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	11	0.22	0.1	0.19
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	11	0.22	0.1	0.19
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	11	0.22	0.09	0.2
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	11	0.22	0.09	0.2
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	11	0.19	0.04	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	11	0.19	0.04	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	11	0.19	0.04	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	11	0.19	0.04	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	11	0.19	0.04	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	11	0.19	0.04	0.18
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	10	2.44	1.32	2.92
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	10	1.21	0.95	1.11
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	10	1.21	0.95	1.11
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	10	0.79	0.41	0.96
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	10	0.79	0.41	0.96
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	10	0.15	0.02	0.16
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	10	0.15	0.02	0.16
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	9	1.66	1.03	1.65
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	9	1.66	1.03	1.65
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	9	1.0	0.62	1.06
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	9	1.0	0.62	1.06
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	9	0.39	0.38	0.2
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	9	0.39	0.38	0.2
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	8	2.51	0.89	2.62
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	8	2.51	0.89	2.62
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	8	2.1	1.24	2.64
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	8	2.04	1.09	2.0
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	8	2.04	1.09	2.0
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	8	2.04	1.09	2.0
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	8	2.04	1.09	2.0
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	8	2.04	1.09	2.0
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	8	2.04	1.09	2.0
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	8	1.37	1.07	1.32
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	8	1.37	1.07	1.32
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	8	1.37	1.07	1.32
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	8	1.37	1.07	1.32
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	8	1.37	1.07	1.32
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	8	1.37	1.07	1.32
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	8	1.31	0.97	1.51
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	7	0.26	0.09	0.28
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	7	0.21	0.08	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB2	6	1.78	1.28	1.86
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB3	6	1.78	1.28	1.86
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD11	6	1.19	0.86	1.28
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD12	6	1.19	0.86	1.28
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD13	6	1.19	0.86	1.28
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD11	6	1.19	0.86	1.28
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD12	6	1.19	0.86	1.28
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD13	6	1.19	0.86	1.28
(2,31)	1:A:30:THR:H	1:B:30:THR:HA	6	0.67	0.53	0.5
(2,31)	1:A:30:THR:H	1:E:30:THR:HA	6	0.67	0.53	0.5
(1,138)	1:A:13:ILE:HA	1:A:16:SER:H	6	0.29	0.1	0.31
(1,366)	1:A:53:LYS:H	1:A:53:LYS:HG2	6	0.2	0.11	0.16
(1,189)	1:A:64:ASN:H	1:A:64:ASN:HB3	6	0.14	0.03	0.14
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG21	5	1.64	0.83	1.36
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG22	5	1.64	0.83	1.36
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG23	5	1.64	0.83	1.36
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG21	5	1.64	0.83	1.36
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG22	5	1.64	0.83	1.36
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG23	5	1.64	0.83	1.36
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD21	5	1.3	0.66	1.41
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD22	5	1.3	0.66	1.41
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD23	5	1.3	0.66	1.41
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD21	5	1.3	0.66	1.41
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD22	5	1.3	0.66	1.41
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD23	5	1.3	0.66	1.41
(2,40)	1:E:30:THR:H	1:A:26:PHE:HB2	5	0.59	0.46	0.36
(2,40)	1:E:30:THR:H	1:D:26:PHE:HB2	5	0.59	0.46	0.36
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH21	5	0.56	0.36	0.43
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH22	5	0.56	0.36	0.43
(2,32)	1:B:30:THR:H	1:A:30:THR:HA	5	0.53	0.67	0.25
(2,32)	1:B:30:THR:H	1:C:30:THR:HA	5	0.53	0.67	0.25
(2,34)	1:D:30:THR:H	1:C:30:THR:HA	5	0.37	0.36	0.2
(2,34)	1:D:30:THR:H	1:E:30:THR:HA	5	0.37	0.36	0.2
(1,152)	1:A:30:THR:HA	1:A:34:LEU:H	5	0.23	0.09	0.17
(1,464)	1:A:45:ASN:HB2	1:A:46:ILE:H	5	0.15	0.04	0.13
(1,464)	1:A:45:ASN:HB3	1:A:46:ILE:H	5	0.15	0.04	0.13
(2,50)	1:E:47:VAL:H	1:D:64:ASN:H	4	2.08	1.15	2.6
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD21	4	1.6	0.51	1.44
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD22	4	1.6	0.51	1.44
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD23	4	1.6	0.51	1.44
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD21	4	1.6	0.51	1.44
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD22	4	1.6	0.51	1.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD23	4	1.6	0.51	1.44
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD11	3	1.78	0.66	2.15
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD12	3	1.78	0.66	2.15
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD13	3	1.78	0.66	2.15
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD11	3	1.78	0.66	2.15
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD12	3	1.78	0.66	2.15
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD13	3	1.78	0.66	2.15
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD21	3	1.51	1.04	1.82
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD22	3	1.51	1.04	1.82
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD23	3	1.51	1.04	1.82
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD21	3	1.51	1.04	1.82
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD22	3	1.51	1.04	1.82
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD23	3	1.51	1.04	1.82
(1,106)	1:A:48:ASN:H	1:A:49:VAL:H	3	0.58	0.14	0.55
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE1	3	0.31	0.11	0.25
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE2	3	0.31	0.11	0.25
(1,230)	1:A:51:LEU:H	1:A:52:VAL:H	3	0.26	0.19	0.13
(2,36)	1:A:30:THR:H	1:B:26:PHE:HB2	3	0.21	0.08	0.18
(2,36)	1:A:30:THR:H	1:E:26:PHE:HB2	3	0.21	0.08	0.18
(1,136)	1:A:55:THR:HB	1:A:56:VAL:H	3	0.19	0.02	0.18
(1,376)	1:A:25:VAL:HB	1:A:26:PHE:H	3	0.19	0.09	0.14
(1,362)	1:A:53:LYS:H	1:A:53:LYS:HG3	3	0.16	0.05	0.14
(2,38)	1:C:30:THR:H	1:B:26:PHE:HB2	3	0.16	0.05	0.14
(2,38)	1:C:30:THR:H	1:D:26:PHE:HB2	3	0.16	0.05	0.14
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG11	2	1.62	0.18	1.62
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG12	2	1.62	0.18	1.62
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG13	2	1.62	0.18	1.62
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG11	2	1.62	0.18	1.62
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG12	2	1.62	0.18	1.62
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG13	2	1.62	0.18	1.62
(1,491)	1:A:61:ARG:HE	1:A:63:LYS:HG2	2	0.96	0.51	0.96
(1,491)	1:A:61:ARG:HE	1:A:63:LYS:HG3	2	0.96	0.51	0.96
(1,120)	1:A:38:ARG:H	1:A:38:ARG:HH21	2	0.6	0.02	0.6
(1,120)	1:A:38:ARG:H	1:A:38:ARG:HH22	2	0.6	0.02	0.6
(1,188)	1:A:62:VAL:HA	1:A:64:ASN:H	2	0.5	0.02	0.5
(1,89)	1:A:23:PHE:HB3	1:A:24:VAL:H	2	0.4	0.0	0.4
(1,429)	1:A:23:PHE:HB2	1:A:24:VAL:H	2	0.26	0.08	0.26
(1,429)	1:A:23:PHE:HB3	1:A:24:VAL:H	2	0.26	0.08	0.26
(1,494)	1:A:62:VAL:HG11	1:A:65:LEU:H	2	0.24	0.06	0.24
(1,494)	1:A:62:VAL:HG12	1:A:65:LEU:H	2	0.24	0.06	0.24
(1,494)	1:A:62:VAL:HG13	1:A:65:LEU:H	2	0.24	0.06	0.24
(1,494)	1:A:62:VAL:HG21	1:A:65:LEU:H	2	0.24	0.06	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,494)	1:A:62:VAL:HG22	1:A:65:LEU:H	2	0.24	0.06	0.24
(1,494)	1:A:62:VAL:HG23	1:A:65:LEU:H	2	0.24	0.06	0.24
(1,275)	1:A:23:PHE:HA	1:A:27:LEU:H	2	0.18	0.06	0.18
(1,74)	1:A:33:ILE:HB	1:A:36:ALA:H	2	0.16	0.04	0.16
(1,343)	1:A:28:LEU:H	1:A:30:THR:H	2	0.14	0.03	0.14
(1,351)	1:A:61:ARG:HB3	1:A:62:VAL:H	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
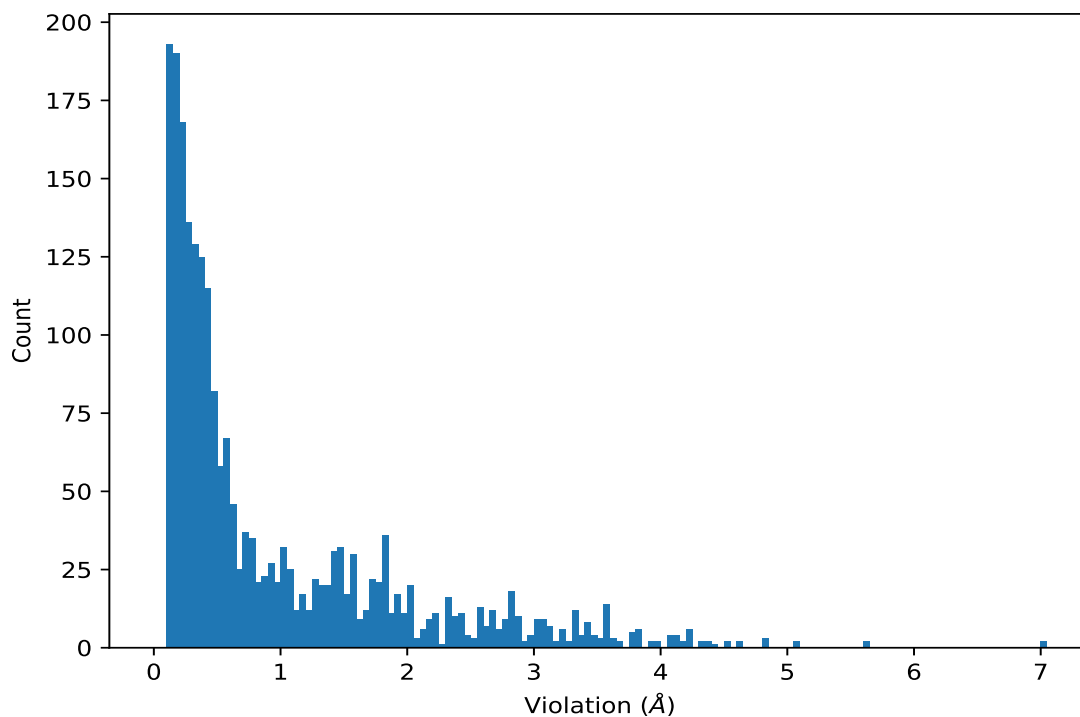
9.5.2 Table : All distance violations ⓘ

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	16	7.05
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	16	7.05
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	15	5.61
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	15	5.61
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	16	5.09
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	16	5.09
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	16	4.82
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	14	4.81
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	14	4.81
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	5	4.62
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	5	4.62
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	10	4.5
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	10	4.5
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	12	4.44
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	14	4.38
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	14	4.38
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	14	4.34
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	14	4.34
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	13	4.22
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	13	4.22
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	15	4.22
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	15	4.22
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	8	4.21
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	8	4.21
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	14	4.18
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	14	4.18
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	8	4.14
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	8	4.14
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	2	4.11
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	2	4.11
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	6	4.09
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	6	4.09
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	12	4.09
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	12	4.09
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	15	3.95
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	15	3.95
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	13	3.92
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	13	3.92
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	11	3.82
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	11	3.82
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	16	3.82
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	16	3.82
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	5	3.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	5	3.81
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	10	3.77
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	11	3.76
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	11	3.76
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	12	3.76
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	12	3.76
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	13	3.65
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	13	3.65
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	8	3.61
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	8	3.61
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	5	3.6
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	7	3.59
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	7	3.59
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	2	3.59
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	2	3.59
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	9	3.58
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	15	3.58
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	8	3.57
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	8	3.57
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	8	3.57
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	8	3.57
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	8	3.57
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	8	3.57
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	8	3.55
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	8	3.55
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB2	10	3.54
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB3	10	3.54
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	16	3.51
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	15	3.49
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	15	3.49
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	6	3.47
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	6	3.47
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	1	3.43
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	11	3.43
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	11	3.43
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	6	3.41
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	6	3.41
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	6	3.41
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	6	3.41
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	6	3.4
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	7	3.37
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	7	3.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	14	3.37
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	14	3.37
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	15	3.34
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	15	3.34
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	15	3.34
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	15	3.34
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	15	3.34
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	15	3.34
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	10	3.33
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	10	3.33
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	4	3.31
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	4	3.31
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	16	3.3
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	16	3.3
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	1	3.28
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	1	3.28
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	7	3.22
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	7	3.22
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	3	3.21
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	3	3.21
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	14	3.2
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	14	3.2
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	15	3.17
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	15	3.17
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	16	3.14
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	16	3.14
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	2	3.13
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	3	3.11
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	3	3.11
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	11	3.1
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	11	3.1
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	15	3.09
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	15	3.09
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	16	3.08
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	16	3.08
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	7	3.08
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	7	3.08
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	11	3.08
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	11	3.08
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	12	3.05
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	2	3.03
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	2	3.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	3	3.03
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	3	3.03
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	16	3.02
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	16	3.02
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	2	3.01
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	2	3.01
(2,50)	1:E:47:VAL:H	1:D:64:ASN:H	4	3.0
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	11	2.99
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	11	2.99
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	11	2.99
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	10	2.95
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	15	2.94
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	15	2.94
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	12	2.89
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	12	2.89
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	16	2.89
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	16	2.89
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	7	2.88
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	7	2.88
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	16	2.86
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	16	2.86
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	1	2.86
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	1	2.86
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	5	2.83
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	5	2.83
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	7	2.83
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	7	2.83
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	8	2.83
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	8	2.83
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	8	2.83
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	8	2.83
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	8	2.83
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	8	2.83
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG21	8	2.83
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG22	8	2.83
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG23	8	2.83
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG21	8	2.83
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG22	8	2.83
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG23	8	2.83
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	5	2.8
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	5	2.8
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	13	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	2	2.75
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	2	2.75
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	15	2.75
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	15	2.75
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	15	2.75
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	15	2.75
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	15	2.75
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	15	2.75
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB2	4	2.73
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB3	4	2.73
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB2	16	2.73
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB3	16	2.73
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	1	2.72
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	1	2.72
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	9	2.69
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	9	2.69
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	5	2.69
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	5	2.69
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	7	2.69
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	7	2.69
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	7	2.69
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	7	2.69
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	7	2.69
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	7	2.69
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	3	2.67
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	3	2.67
(2,50)	1:E:47:VAL:H	1:D:64:ASN:H	16	2.63
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD21	7	2.6
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD22	7	2.6
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD23	7	2.6
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD21	7	2.6
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD22	7	2.6
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD23	7	2.6
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	7	2.59
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	9	2.59
(2,50)	1:E:47:VAL:H	1:D:64:ASN:H	10	2.58
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD11	15	2.57
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD12	15	2.57
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD13	15	2.57
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD11	15	2.57
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD12	15	2.57
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD13	15	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	8	2.56
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	8	2.56
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	10	2.55
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	10	2.55
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	4	2.53
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	3	2.51
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	3	2.51
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	8	2.48
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	8	2.48
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	2	2.47
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	2	2.47
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	13	2.44
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	13	2.44
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	13	2.42
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	13	2.42
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD21	7	2.42
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD22	7	2.42
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD23	7	2.42
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD21	7	2.42
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD22	7	2.42
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD23	7	2.42
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	11	2.41
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	10	2.39
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	10	2.39
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	6	2.38
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	6	2.38
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	2	2.37
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	2	2.37
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	4	2.37
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	4	2.37
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	9	2.35
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	9	2.35
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	1	2.33
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	1	2.33
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD11	8	2.33
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD12	8	2.33
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD13	8	2.33
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD11	8	2.33
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD12	8	2.33
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD13	8	2.33
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	1	2.32
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	1	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG21	15	2.3
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG22	15	2.3
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG23	15	2.3
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG21	15	2.3
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG22	15	2.3
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG23	15	2.3
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	4	2.25
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	16	2.24
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	16	2.24
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	16	2.24
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	16	2.24
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	16	2.24
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	16	2.24
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	15	2.24
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	15	2.22
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	15	2.22
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	12	2.22
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	12	2.22
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	8	2.18
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	4	2.16
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	4	2.16
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD11	15	2.15
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD12	15	2.15
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD13	15	2.15
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD11	15	2.15
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD12	15	2.15
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD13	15	2.15
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	15	2.14
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	15	2.14
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	15	2.13
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	15	2.13
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	13	2.12
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	13	2.12
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	4	2.06
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	4	2.06
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	12	2.05
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	9	2.04
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	9	2.04
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	5	2.03
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	5	2.03
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	16	2.03
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	16	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	16	2.03
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	16	2.03
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	16	2.03
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	16	2.03
(2,15)	1:E:16:SER:H	1:A:12:LEU:HD11	7	2.02
(2,15)	1:E:16:SER:H	1:A:12:LEU:HD12	7	2.02
(2,15)	1:E:16:SER:H	1:A:12:LEU:HD13	7	2.02
(2,15)	1:E:16:SER:H	1:D:12:LEU:HD11	7	2.02
(2,15)	1:E:16:SER:H	1:D:12:LEU:HD12	7	2.02
(2,15)	1:E:16:SER:H	1:D:12:LEU:HD13	7	2.02
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	14	2.01
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	14	2.01
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	9	2.0
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	9	2.0
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	6	1.99
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	6	1.99
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD21	14	1.98
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD22	14	1.98
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD23	14	1.98
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD21	14	1.98
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD22	14	1.98
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD23	14	1.98
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	1	1.98
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	13	1.97
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	13	1.97
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	11	1.93
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	1	1.93
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	1	1.93
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	11	1.93
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	11	1.93
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	11	1.93
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	11	1.93
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	11	1.93
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	11	1.93
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	1	1.93
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	1	1.93
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	12	1.91
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	12	1.91
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	6	1.9
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	6	1.9
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	8	1.9
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	8	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	15	1.88
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	15	1.88
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	10	1.88
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	10	1.88
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	10	1.87
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	10	1.87
(2,32)	1:B:30:THR:H	1:A:30:THR:HA	14	1.87
(2,32)	1:B:30:THR:H	1:C:30:THR:HA	14	1.87
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	8	1.87
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	13	1.86
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	13	1.86
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	2	1.84
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	2	1.84
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	6	1.83
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	6	1.83
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	8	1.83
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	8	1.83
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	9	1.83
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	9	1.83
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	8	1.82
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	8	1.82
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	4	1.82
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	4	1.82
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD21	15	1.82
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD22	15	1.82
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD23	15	1.82
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD21	15	1.82
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD22	15	1.82
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD23	15	1.82
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	2	1.82
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	11	1.82
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD21	9	1.81
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD22	9	1.81
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD23	9	1.81
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD21	9	1.81
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD22	9	1.81
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD23	9	1.81
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	14	1.81
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	14	1.81
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	13	1.81
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG11	8	1.8
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG12	8	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG13	8	1.8
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG11	8	1.8
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG12	8	1.8
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG13	8	1.8
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	9	1.8
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	11	1.79
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	11	1.79
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	11	1.79
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	11	1.79
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	2	1.79
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	2	1.79
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	2	1.79
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	2	1.79
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	2	1.79
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	2	1.79
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	6	1.77
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	12	1.76
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	12	1.76
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	13	1.76
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	13	1.76
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	13	1.76
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	13	1.76
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	13	1.76
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	13	1.76
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	7	1.76
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	7	1.76
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	14	1.74
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	14	1.74
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	14	1.74
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	14	1.74
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	14	1.74
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	14	1.74
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	14	1.74
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB2	1	1.73
(2,44)	1:D:39:LEU:H	1:C:57:TYR:HB3	1	1.73
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	9	1.73
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	9	1.73
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	12	1.72
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	12	1.72
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	8	1.71
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD11	7	1.7
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD12	7	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD13	7	1.7
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD11	7	1.7
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD12	7	1.7
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD13	7	1.7
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	3	1.7
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	3	1.7
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	1	1.69
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	1	1.69
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	1	1.69
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	1	1.69
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	1	1.69
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	1	1.69
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	8	1.66
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	5	1.66
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	5	1.66
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	7	1.66
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	13	1.65
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	13	1.65
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	12	1.64
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	5	1.62
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	5	1.62
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD21	9	1.62
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD22	9	1.62
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD23	9	1.62
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD21	9	1.62
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD22	9	1.62
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD23	9	1.62
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD11	8	1.58
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD12	8	1.58
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD13	8	1.58
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD11	8	1.58
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD12	8	1.58
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD13	8	1.58
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	5	1.58
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	5	1.58
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	5	1.58
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	5	1.58
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	5	1.58
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	5	1.58
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	12	1.58
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	12	1.58
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	12	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	12	1.58
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	12	1.58
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	12	1.58
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	10	1.57
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	10	1.57
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	10	1.57
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	10	1.57
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	10	1.57
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	10	1.57
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	3	1.57
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	11	1.56
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	11	1.56
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	5	1.56
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	8	1.55
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	8	1.55
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	11	1.54
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	11	1.54
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	3	1.52
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	3	1.52
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	3	1.52
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	3	1.52
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	3	1.52
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	3	1.52
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	12	1.51
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	12	1.51
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	11	1.51
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	11	1.51
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	16	1.51
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	16	1.51
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	14	1.5
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	15	1.5
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	15	1.5
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	12	1.48
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	12	1.48
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	4	1.48
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	4	1.48
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	15	1.48
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	15	1.48
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	15	1.48
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	15	1.48
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	15	1.48
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	15	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	14	1.47
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	14	1.47
(1,491)	1:A:61:ARG:HE	1:A:63:LYS:HG2	14	1.47
(1,491)	1:A:61:ARG:HE	1:A:63:LYS:HG3	14	1.47
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	4	1.46
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	4	1.46
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	4	1.46
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	4	1.46
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	4	1.46
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	4	1.46
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG11	15	1.45
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG12	15	1.45
(2,5)	1:E:14:VAL:H	1:A:14:VAL:HG13	15	1.45
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG11	15	1.45
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG12	15	1.45
(2,5)	1:E:14:VAL:H	1:D:14:VAL:HG13	15	1.45
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	11	1.45
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	11	1.45
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	11	1.45
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	11	1.45
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	11	1.45
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	11	1.45
(2,31)	1:A:30:THR:H	1:B:30:THR:HA	16	1.44
(2,31)	1:A:30:THR:H	1:E:30:THR:HA	16	1.44
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	10	1.44
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	10	1.44
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	16	1.44
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	16	1.44
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	16	1.44
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	16	1.44
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	16	1.44
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	16	1.44
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	7	1.43
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	7	1.43
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	7	1.43
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	7	1.43
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	7	1.43
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	7	1.43
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	12	1.42
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	12	1.42
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	9	1.42
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	9	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	9	1.42
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	9	1.42
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	9	1.42
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	9	1.42
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD21	6	1.41
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD22	6	1.41
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD23	6	1.41
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD21	6	1.41
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD22	6	1.41
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD23	6	1.41
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	16	1.4
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	7	1.38
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	7	1.38
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	4	1.38
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	4	1.38
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	4	1.38
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	4	1.38
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	8	1.38
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	8	1.38
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	8	1.38
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	8	1.38
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	8	1.38
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	8	1.38
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	2	1.38
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	15	1.36
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG21	16	1.36
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG22	16	1.36
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG23	16	1.36
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG21	16	1.36
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG22	16	1.36
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG23	16	1.36
(2,40)	1:E:30:THR:H	1:A:26:PHE:HB2	4	1.34
(2,40)	1:E:30:THR:H	1:D:26:PHE:HB2	4	1.34
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	1	1.34
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	1	1.34
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	7	1.31
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	7	1.31
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	13	1.31
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	13	1.31
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	13	1.31
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	13	1.31
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	13	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	13	1.31
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	10	1.3
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	10	1.3
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	15	1.3
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	15	1.3
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	15	1.3
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	15	1.3
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	2	1.3
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	2	1.3
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	6	1.29
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	6	1.29
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	6	1.29
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	6	1.29
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	6	1.29
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	6	1.29
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD21	5	1.27
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD22	5	1.27
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD23	5	1.27
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD21	5	1.27
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD22	5	1.27
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD23	5	1.27
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH21	14	1.27
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH22	14	1.27
(2,31)	1:A:30:THR:H	1:B:30:THR:HA	5	1.26
(2,31)	1:A:30:THR:H	1:E:30:THR:HA	5	1.26
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG21	9	1.26
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG22	9	1.26
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG23	9	1.26
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG21	9	1.26
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG22	9	1.26
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG23	9	1.26
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	6	1.24
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	6	1.24
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	12	1.23
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	11	1.23
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	11	1.23
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	9	1.21
(1,455)	1:A:37:LEU:HD11	1:A:40:ALA:H	1	1.2
(1,455)	1:A:37:LEU:HD12	1:A:40:ALA:H	1	1.2
(1,455)	1:A:37:LEU:HD13	1:A:40:ALA:H	1	1.2
(1,455)	1:A:37:LEU:HD21	1:A:40:ALA:H	1	1.2
(1,455)	1:A:37:LEU:HD22	1:A:40:ALA:H	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:37:LEU:HD23	1:A:40:ALA:H	1	1.2
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD21	12	1.19
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD22	12	1.19
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD23	12	1.19
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD21	12	1.19
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD22	12	1.19
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD23	12	1.19
(1,503)	1:A:64:ASN:HD21	1:A:65:LEU:HA	10	1.18
(1,503)	1:A:64:ASN:HD22	1:A:65:LEU:HA	10	1.18
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	1	1.18
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	1	1.18
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	6	1.18
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	16	1.16
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	16	1.16
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	4	1.16
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	3	1.15
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	3	1.15
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	3	1.15
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	1	1.14
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	1	1.14
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	1	1.14
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	1	1.14
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	10	1.12
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	10	1.12
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	1	1.12
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	2	1.12
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	14	1.1
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	14	1.1
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	8	1.1
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	8	1.1
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	7	1.09
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	7	1.09
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	13	1.09
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	2	1.08
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	2	1.08
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	6	1.08
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	6	1.08
(2,34)	1:D:30:THR:H	1:C:30:THR:HA	14	1.08
(2,34)	1:D:30:THR:H	1:E:30:THR:HA	14	1.08
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD21	4	1.08
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD22	4	1.08
(2,17)	1:B:16:SER:H	1:A:12:LEU:HD23	4	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD21	4	1.08
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD22	4	1.08
(2,17)	1:B:16:SER:H	1:C:12:LEU:HD23	4	1.08
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	13	1.08
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	13	1.08
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	14	1.07
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	14	1.06
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	14	1.06
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	13	1.06
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	4	1.05
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	4	1.05
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	9	1.05
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	9	1.05
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	2	1.04
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	2	1.04
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	11	1.04
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	11	1.04
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	14	1.04
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	14	1.04
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	3	1.04
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	3	1.04
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	8	1.03
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	8	1.03
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	8	1.03
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	8	1.03
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	12	1.03
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	16	1.03
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	9	1.02
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	9	1.02
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	9	1.02
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	9	1.02
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	10	1.02
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	10	1.02
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	12	1.02
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	12	1.02
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	10	1.02
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	3	1.01
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB2	12	1.0
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB3	12	1.0
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	4	1.0
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	4	1.0
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	6	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	6	1.0
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	12	1.0
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	12	1.0
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	9	0.99
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	9	0.99
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD11	16	0.98
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD12	16	0.98
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD13	16	0.98
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD11	16	0.98
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD12	16	0.98
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD13	16	0.98
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	2	0.98
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	2	0.98
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	2	0.98
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	2	0.98
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	2	0.98
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	4	0.97
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	2	0.95
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	2	0.95
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB2	13	0.95
(2,42)	1:B:39:LEU:H	1:A:57:TYR:HB3	13	0.95
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	14	0.95
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	14	0.95
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	8	0.95
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	14	0.94
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	14	0.94
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	12	0.94
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	5	0.93
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	5	0.93
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	6	0.93
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	6	0.93
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	6	0.93
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	14	0.93
(1,175)	1:A:64:ASN:HD22	1:A:65:LEU:H	10	0.93
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	15	0.92
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	15	0.92
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	12	0.92
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	12	0.92
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	6	0.91
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	6	0.91
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	6	0.91
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	6	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	1:E:30:THR:H	1:A:26:PHE:HB2	3	0.9
(2,40)	1:E:30:THR:H	1:D:26:PHE:HB2	3	0.9
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	11	0.9
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	11	0.9
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	11	0.9
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	11	0.9
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	4	0.9
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	4	0.9
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	3	0.9
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	7	0.88
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	7	0.88
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	7	0.88
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	7	0.88
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	13	0.88
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	13	0.88
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	13	0.88
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	13	0.88
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	5	0.88
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	9	0.86
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	7	0.86
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	7	0.86
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	3	0.86
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD11	16	0.85
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD12	16	0.85
(2,11)	1:A:16:SER:H	1:B:12:LEU:HD13	16	0.85
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD11	16	0.85
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD12	16	0.85
(2,11)	1:A:16:SER:H	1:E:12:LEU:HD13	16	0.85
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	12	0.85
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	12	0.85
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	12	0.85
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	12	0.85
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	16	0.84
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	12	0.83
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	12	0.83
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	13	0.83
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	13	0.83
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB2	6	0.82
(2,43)	1:C:39:LEU:H	1:B:57:TYR:HB3	6	0.82
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	4	0.82
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	2	0.82
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	12	0.81
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	15	0.81
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	3	0.81
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	3	0.81
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	3	0.81
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	3	0.81
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	15	0.81
(2,31)	1:A:30:THR:H	1:B:30:THR:HA	11	0.8
(2,31)	1:A:30:THR:H	1:E:30:THR:HA	11	0.8
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	12	0.8
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	15	0.8
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	5	0.79
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	5	0.79
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	2	0.78
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	2	0.78
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	2	0.78
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	4	0.78
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	4	0.78
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	4	0.78
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	1	0.78
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	14	0.78
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	16	0.77
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	3	0.77
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	3	0.77
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	5	0.77
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	11	0.77
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	8	0.77
(1,106)	1:A:48:ASN:H	1:A:49:VAL:H	13	0.77
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	1	0.76
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	1	0.76
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	1	0.76
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	12	0.76
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	12	0.76
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	10	0.76
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	10	0.75
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	10	0.75
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	11	0.75
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	11	0.75
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	13	0.75
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	13	0.75
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	15	0.75
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	15	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	7	0.75
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	14	0.75
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	14	0.75
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	14	0.75
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	3	0.74
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	3	0.74
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	3	0.74
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	5	0.74
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	5	0.74
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	10	0.74
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	2	0.74
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	10	0.74
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	4	0.74
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	16	0.74
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	3	0.73
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	16	0.73
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	16	0.73
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	9	0.72
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	9	0.72
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	14	0.72
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	14	0.72
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	8	0.72
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	11	0.71
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	5	0.71
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	5	0.71
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	5	0.71
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	5	0.71
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	7	0.71
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	7	0.71
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	16	0.71
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	15	0.71
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	5	0.7
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	5	0.7
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	5	0.7
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	5	0.7
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	5	0.7
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	5	0.7
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	2	0.7
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	2	0.7
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	2	0.7
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	14	0.7
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	4	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	4	0.69
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	4	0.69
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	6	0.69
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	6	0.69
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	8	0.68
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	8	0.68
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	7	0.68
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	9	0.68
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	16	0.67
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	9	0.67
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	15	0.66
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	15	0.66
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB2	3	0.66
(1,457)	1:A:39:LEU:H	1:A:39:LEU:HB3	3	0.66
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	2	0.66
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	13	0.65
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	13	0.65
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	13	0.65
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	15	0.65
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	9	0.65
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	9	0.65
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	9	0.65
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	14	0.65
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	5	0.65
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	14	0.64
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	14	0.64
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	14	0.64
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	14	0.64
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	11	0.64
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	13	0.64
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	7	0.63
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	14	0.63
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	14	0.63
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	14	0.63
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	14	0.63
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	3	0.63
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	8	0.63
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	2	0.63
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	2	0.63
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	2	0.63
(2,26)	1:A:28:LEU:H	1:B:24:VAL:HA	4	0.62
(2,26)	1:A:28:LEU:H	1:E:24:VAL:HA	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	9	0.62
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	9	0.62
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	9	0.62
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	9	0.62
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	9	0.62
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	9	0.62
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	10	0.62
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	3	0.62
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	3	0.62
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	3	0.62
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	11	0.62
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	13	0.62
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	15	0.62
(1,120)	1:A:38:ARG:H	1:A:38:ARG:HH21	3	0.62
(1,120)	1:A:38:ARG:H	1:A:38:ARG:HH22	3	0.62
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	4	0.61
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	9	0.61
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	11	0.61
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	15	0.61
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	6	0.61
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	9	0.6
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	9	0.6
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	9	0.6
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	15	0.6
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	3	0.6
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	3	0.6
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	3	0.6
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	3	0.6
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	14	0.59
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	1	0.59
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	2	0.59
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	3	0.59
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	6	0.59
(1,120)	1:A:38:ARG:H	1:A:38:ARG:HH21	6	0.59
(1,120)	1:A:38:ARG:H	1:A:38:ARG:HH22	6	0.59
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	4	0.59
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	6	0.59
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	6	0.58
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	6	0.58
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	7	0.58
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	7	0.58
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:A:64:ASN:HD21	1:A:65:LEU:H	16	0.58
(1,502)	1:A:64:ASN:HD22	1:A:65:LEU:H	16	0.58
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	3	0.58
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	3	0.58
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	3	0.58
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	3	0.58
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	3	0.58
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	3	0.58
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	6	0.58
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	4	0.58
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	5	0.57
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	5	0.57
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	5	0.57
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	8	0.57
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	8	0.57
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	8	0.57
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	14	0.57
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	14	0.57
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	14	0.57
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	8	0.57
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	7	0.57
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	7	0.57
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	7	0.57
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	16	0.57
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	11	0.57
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	9	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	9	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	9	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	9	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	9	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	9	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	14	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	14	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	14	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	14	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	14	0.56
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	14	0.56
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	5	0.56
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	5	0.56
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	11	0.56
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	13	0.56
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	13	0.56
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	16	0.56
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	16	0.56
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	16	0.56
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	10	0.56
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	2	0.55
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	2	0.55
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	2	0.55
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	11	0.55
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	1	0.55
(1,106)	1:A:48:ASN:H	1:A:49:VAL:H	5	0.55
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB2	11	0.54
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB3	11	0.54
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	6	0.54
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	6	0.54
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	6	0.54
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	8	0.54
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	13	0.54
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	12	0.54
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	12	0.54
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	10	0.54
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	10	0.54
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	10	0.54
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	10	0.54
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	10	0.54
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	10	0.54
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	1	0.54
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	4	0.54
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	7	0.54
(1,114)	1:A:38:ARG:H	1:A:40:ALA:H	13	0.54
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	2	0.53
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	7	0.53
(1,230)	1:A:51:LEU:H	1:A:52:VAL:H	8	0.53
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	6	0.53
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	14	0.53
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	8	0.52
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	13	0.52
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	15	0.52
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	1	0.52
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	1	0.52
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	1	0.52
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	11	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	11	0.52
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	11	0.52
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	12	0.52
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	12	0.52
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	12	0.52
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	13	0.52
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	13	0.52
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	13	0.52
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	13	0.52
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	13	0.52
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	13	0.52
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	8	0.52
(1,188)	1:A:62:VAL:HA	1:A:64:ASN:H	4	0.52
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	9	0.51
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	9	0.51
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	1	0.51
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	1	0.51
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	1	0.51
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	15	0.51
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	15	0.51
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	15	0.51
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	10	0.5
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	12	0.5
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	9	0.5
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	12	0.5
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	12	0.5
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	12	0.5
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	10	0.49
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	10	0.49
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	10	0.49
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	2	0.49
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	2	0.49
(1,188)	1:A:62:VAL:HA	1:A:64:ASN:H	16	0.49
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	16	0.49
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	11	0.48
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	6	0.48
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	6	0.48
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	14	0.48
(1,28)	1:A:54:PRO:HG2	1:A:55:THR:H	5	0.48
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	15	0.48
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	15	0.48
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	15	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	5	0.48
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	16	0.47
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	16	0.47
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	16	0.47
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE1	2	0.47
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE2	2	0.47
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	7	0.47
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	12	0.47
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	3	0.47
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	10	0.47
(2,29)	1:D:28:LEU:H	1:C:24:VAL:HA	4	0.46
(2,29)	1:D:28:LEU:H	1:E:24:VAL:HA	4	0.46
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	1	0.46
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	1	0.46
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	1	0.46
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	1	0.46
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	1	0.46
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	1	0.46
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG21	11	0.46
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG22	11	0.46
(2,10)	1:E:14:VAL:H	1:A:14:VAL:HG23	11	0.46
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG21	11	0.46
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG22	11	0.46
(2,10)	1:E:14:VAL:H	1:D:14:VAL:HG23	11	0.46
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB2	16	0.46
(1,504)	1:A:64:ASN:HD21	1:A:65:LEU:HB3	16	0.46
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB2	16	0.46
(1,504)	1:A:64:ASN:HD22	1:A:65:LEU:HB3	16	0.46
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	3	0.46
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	3	0.46
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH21	6	0.46
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH22	6	0.46
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	1	0.46
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	12	0.46
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	9	0.46
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	9	0.46
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	9	0.46
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	16	0.46
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	16	0.46
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	16	0.46
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	10	0.45
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	11	0.45
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	11	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	1	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	1	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	1	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	1	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	1	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	1	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	15	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	15	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	15	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	15	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	15	0.45
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	15	0.45
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	16	0.45
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	16	0.45
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	10	0.45
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	10	0.45
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	10	0.45
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	1	0.45
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	1	0.45
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	1	0.45
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	13	0.45
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	13	0.45
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	13	0.45
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	5	0.44
(1,72)	1:A:33:ILE:HG21	1:A:36:ALA:H	15	0.44
(1,72)	1:A:33:ILE:HG22	1:A:36:ALA:H	15	0.44
(1,72)	1:A:33:ILE:HG23	1:A:36:ALA:H	15	0.44
(1,491)	1:A:61:ARG:HE	1:A:63:LYS:HG2	4	0.44
(1,491)	1:A:61:ARG:HE	1:A:63:LYS:HG3	4	0.44
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	6	0.44
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	6	0.44
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	6	0.44
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	6	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	7	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	7	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	7	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	7	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	7	0.44
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	7	0.44
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	1	0.44
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	7	0.44
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	7	0.44
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	7	0.44
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	8	0.44
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	8	0.44
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	8	0.44
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	14	0.43
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	14	0.43
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	7	0.43
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	7	0.43
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	16	0.43
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	16	0.43
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	16	0.43
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	16	0.43
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	16	0.43
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	16	0.43
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	9	0.43
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	9	0.43
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH21	2	0.43
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH22	2	0.43
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	8	0.43
(1,366)	1:A:53:LYS:H	1:A:53:LYS:HG2	10	0.43
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	12	0.43
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	12	0.43
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	15	0.43
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	15	0.43
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	1	0.43
(1,149)	1:A:32:ALA:H	1:A:34:LEU:H	2	0.43
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	3	0.43
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	6	0.42
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	10	0.42
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	10	0.42
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	10	0.42
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	10	0.42
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	10	0.42
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	10	0.42
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	12	0.42
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	10	0.42
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	10	0.42
(1,106)	1:A:48:ASN:H	1:A:49:VAL:H	10	0.42
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	4	0.42
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	4	0.42
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	11	0.42
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	11	0.42
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	11	0.42
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	12	0.41
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	12	0.41
(1,89)	1:A:23:PHE:HB3	1:A:24:VAL:H	16	0.41
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	12	0.41
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	12	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	6	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	6	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	6	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	6	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	6	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	6	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	9	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	9	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	9	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	9	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	9	0.41
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	9	0.41
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	6	0.41
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	10	0.41
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	14	0.41
(1,138)	1:A:13:ILE:HA	1:A:16:SER:H	1	0.41
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	16	0.41
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	16	0.41
(1,89)	1:A:23:PHE:HB3	1:A:24:VAL:H	7	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	6	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	6	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	6	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	6	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	6	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	6	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	12	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	12	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	12	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	12	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	12	0.4
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	12	0.4
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	10	0.4
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	11	0.4
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	11	0.4
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	16	0.4
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	12	0.4
(1,173)	1:A:61:ARG:H	1:A:61:ARG:HE	14	0.4
(1,170)	1:A:61:ARG:HE	1:A:64:ASN:H	14	0.4
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	1	0.4
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	1	0.4
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	5	0.4
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	5	0.4
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	5	0.4
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	5	0.4
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	5	0.4
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	16	0.39
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	16	0.39
(2,27)	1:B:28:LEU:H	1:A:24:VAL:HA	9	0.39
(2,27)	1:B:28:LEU:H	1:C:24:VAL:HA	9	0.39
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD21	14	0.39
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD22	14	0.39
(2,18)	1:C:16:SER:H	1:B:12:LEU:HD23	14	0.39
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD21	14	0.39
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD22	14	0.39
(2,18)	1:C:16:SER:H	1:D:12:LEU:HD23	14	0.39
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	9	0.39
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	10	0.39
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	10	0.39
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	8	0.39
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	8	0.39
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	8	0.39
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	8	0.39
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	8	0.39
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	8	0.39
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	7	0.39
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	7	0.39
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	7	0.39
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	7	0.39
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	7	0.39
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	7	0.39
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	14	0.39
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	14	0.39
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	15	0.39
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	4	0.38
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	4	0.38
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	16	0.38
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	16	0.38
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	4	0.38
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	4	0.38
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	4	0.38
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	4	0.38
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	4	0.38
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	4	0.38
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	8	0.38
(1,152)	1:A:30:THR:HA	1:A:34:LEU:H	8	0.38
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	13	0.37
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	13	0.37
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	5	0.37
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	5	0.37
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	5	0.37
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	5	0.37
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	5	0.37
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	5	0.37
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	12	0.37
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	5	0.37
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	5	0.37
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	11	0.37
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	13	0.37
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	1	0.37
(1,138)	1:A:13:ILE:HA	1:A:16:SER:H	7	0.37
(1,138)	1:A:13:ILE:HA	1:A:16:SER:H	16	0.37
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	1	0.37
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	1	0.37
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	10	0.37
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	10	0.37
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	10	0.37
(2,40)	1:E:30:THR:H	1:A:26:PHE:HB2	14	0.36
(2,40)	1:E:30:THR:H	1:D:26:PHE:HB2	14	0.36
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	9	0.36
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	9	0.36
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	2	0.36
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	2	0.36
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	7	0.36
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	9	0.36
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	9	0.36
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	11	0.36
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	11	0.36
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	10	0.36
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	10	0.36
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	15	0.36
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	15	0.36
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	7	0.36
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	7	0.36
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH21	3	0.36
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH22	3	0.36
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	10	0.36
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	10	0.36
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	13	0.36
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	13	0.36
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	9	0.36
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	13	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	1	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	1	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	1	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	5	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	5	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	5	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	12	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	12	0.36
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	12	0.36
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	8	0.36
(1,105)	1:A:47:VAL:HG21	1:A:48:ASN:H	6	0.36
(1,105)	1:A:47:VAL:HG22	1:A:48:ASN:H	6	0.36
(1,105)	1:A:47:VAL:HG23	1:A:48:ASN:H	6	0.36
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	14	0.35
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	16	0.35
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	13	0.35
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	13	0.35
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	15	0.35
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	15	0.35
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	11	0.35
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	11	0.35
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	11	0.35
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	11	0.35
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	11	0.35
(1,429)	1:A:23:PHE:HB2	1:A:24:VAL:H	7	0.35
(1,429)	1:A:23:PHE:HB3	1:A:24:VAL:H	7	0.35
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	2	0.35
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	3	0.35
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	6	0.35
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	8	0.35
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	8	0.35
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	8	0.35
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	5	0.35
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	13	0.35
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	7	0.35
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	13	0.35
(2,34)	1:D:30:THR:H	1:C:30:THR:HA	15	0.34
(2,34)	1:D:30:THR:H	1:E:30:THR:HA	15	0.34
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	10	0.34
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	10	0.34
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	4	0.34
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	1	0.34
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	1	0.34
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	2	0.34
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	2	0.34
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	8	0.34
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	8	0.34
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	5	0.34
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	5	0.34
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	3	0.34
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	3	0.34
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	3	0.34
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	3	0.34
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	3	0.34
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	3	0.34
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	4	0.34
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	4	0.34
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	1	0.34
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	7	0.34
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	3	0.34
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	5	0.34
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	11	0.34
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	11	0.34
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	3	0.33
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	16	0.33
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	3	0.33
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	5	0.33
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	9	0.33
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	2	0.33
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	6	0.33
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	5	0.33
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	11	0.33
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	7	0.33
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	7	0.33
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	16	0.32
(2,36)	1:A:30:THR:H	1:B:26:PHE:HB2	7	0.32
(2,36)	1:A:30:THR:H	1:E:26:PHE:HB2	7	0.32
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	3	0.32
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	1	0.32
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	1	0.32
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	6	0.32
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	6	0.32
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	3	0.32
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	3	0.32
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	9	0.32
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	7	0.32
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	11	0.32
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	6	0.32
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	6	0.32
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	6	0.32
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	13	0.32
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	14	0.32
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	4	0.32
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	4	0.32
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	11	0.32
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	7	0.32
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	7	0.32
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	14	0.32
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	14	0.32
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	12	0.31
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	3	0.31
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	3	0.31
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	4	0.31
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	4	0.31
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	15	0.31
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:A:54:PRO:HB2	1:A:55:THR:H	5	0.31
(1,479)	1:A:54:PRO:HB3	1:A:55:THR:H	5	0.31
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	12	0.31
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	12	0.31
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD11	2	0.31
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD12	2	0.31
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD13	2	0.31
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD21	2	0.31
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD22	2	0.31
(1,447)	1:A:31:LEU:H	1:A:31:LEU:HD23	2	0.31
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	1	0.31
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	1	0.31
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	11	0.31
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	11	0.31
(1,376)	1:A:25:VAL:HB	1:A:26:PHE:H	8	0.31
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	4	0.31
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	7	0.31
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	1	0.31
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	12	0.31
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	2	0.31
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	4	0.31
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	4	0.31
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	4	0.31
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	11	0.31
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	16	0.31
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	9	0.31
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	10	0.31
(1,152)	1:A:30:THR:HA	1:A:34:LEU:H	3	0.31
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	9	0.31
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	14	0.31
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	8	0.31
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	8	0.31
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	9	0.31
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	9	0.31
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	1	0.31
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	2	0.31
(2,47)	1:B:47:VAL:H	1:A:64:ASN:H	4	0.3
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	4	0.3
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	9	0.3
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	9	0.3
(1,494)	1:A:62:VAL:HG11	1:A:65:LEU:H	10	0.3
(1,494)	1:A:62:VAL:HG12	1:A:65:LEU:H	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:A:62:VAL:HG13	1:A:65:LEU:H	10	0.3
(1,494)	1:A:62:VAL:HG21	1:A:65:LEU:H	10	0.3
(1,494)	1:A:62:VAL:HG22	1:A:65:LEU:H	10	0.3
(1,494)	1:A:62:VAL:HG23	1:A:65:LEU:H	10	0.3
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	4	0.3
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	11	0.3
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	11	0.3
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	11	0.3
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	2	0.3
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	6	0.3
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	11	0.3
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	7	0.3
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	12	0.3
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	7	0.3
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	7	0.3
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	7	0.3
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	10	0.29
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	5	0.29
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	5	0.29
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	13	0.29
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	13	0.29
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	9	0.29
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	9	0.29
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	16	0.29
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	16	0.29
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	1	0.29
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	6	0.29
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	3	0.29
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	16	0.29
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	16	0.29
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	16	0.29
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	11	0.28
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	11	0.28
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	12	0.28
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	7	0.28
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	1	0.28
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	1	0.28
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	1	0.28
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	1	0.28
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	1	0.28
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	1	0.28
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	10	0.28
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	16	0.28
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	16	0.28
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	8	0.28
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	6	0.28
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	10	0.28
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	1	0.28
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	8	0.28
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	14	0.28
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	15	0.28
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	3	0.28
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	3	0.28
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	3	0.28
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	3	0.28
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	1	0.27
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	1	0.27
(2,33)	1:C:30:THR:H	1:B:30:THR:HA	1	0.27
(2,33)	1:C:30:THR:H	1:D:30:THR:HA	1	0.27
(2,32)	1:B:30:THR:H	1:A:30:THR:HA	15	0.27
(2,32)	1:B:30:THR:H	1:C:30:THR:HA	15	0.27
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	5	0.27
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	5	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	14	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	14	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	14	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	14	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	14	0.27
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	14	0.27
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	16	0.27
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	16	0.27
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH21	12	0.27
(1,382)	1:A:61:ARG:H	1:A:61:ARG:HH22	12	0.27
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	3	0.27
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	10	0.27
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	1	0.27
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	1	0.27
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	8	0.27
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	8	0.27
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	13	0.27
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	2	0.27
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	4	0.27
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	3	0.27
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	6	0.27
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	16	0.27
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	5	0.27
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	5	0.27
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	11	0.26
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	11	0.26
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	11	0.26
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	11	0.26
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	1	0.26
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	1	0.26
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	8	0.26
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	8	0.26
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	12	0.26
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	12	0.26
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	14	0.26
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	6	0.26
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	4	0.26
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	10	0.26
(1,198)	1:A:20:PHE:H	1:A:20:PHE:HE1	2	0.26
(1,198)	1:A:20:PHE:H	1:A:20:PHE:HE2	2	0.26
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	7	0.26
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	3	0.26
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	3	0.26
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	4	0.26
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	4	0.26
(1,107)	1:A:48:ASN:H	1:A:50:SER:H	9	0.26
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	3	0.25
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	3	0.25
(2,32)	1:B:30:THR:H	1:A:30:THR:HA	13	0.25
(2,32)	1:B:30:THR:H	1:C:30:THR:HA	13	0.25
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	8	0.25
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	15	0.25
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	8	0.25
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	8	0.25
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	1	0.25
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	1	0.25
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	1	0.25
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	1	0.25
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	1	0.25
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	1	0.25
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	13	0.25
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	13	0.25
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	13	0.25
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	13	0.25
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	13	0.25
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	11	0.25
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	11	0.25
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	4	0.25
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE1	4	0.25
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE2	4	0.25
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	9	0.25
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	5	0.25
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	9	0.25
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	15	0.25
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	14	0.25
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	10	0.25
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	2	0.25
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	2	0.25
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	2	0.25
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	5	0.25
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	8	0.25
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	11	0.25
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	16	0.25
(1,138)	1:A:13:ILE:HA	1:A:16:SER:H	2	0.25
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	13	0.25
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	13	0.25
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	15	0.24
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	1	0.24
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	11	0.24
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	12	0.24
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	7	0.24
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	7	0.24
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	4	0.24
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	4	0.24
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	4	0.24
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	4	0.24
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	4	0.24
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	4	0.24
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	11	0.24
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	11	0.24
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	11	0.24
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	11	0.24
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	11	0.24
(1,403)	1:A:8:GLU:HB2	1:A:11:THR:H	6	0.24
(1,403)	1:A:8:GLU:HB3	1:A:11:THR:H	6	0.24
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	3	0.24
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	3	0.24
(1,366)	1:A:53:LYS:H	1:A:53:LYS:HG2	12	0.24
(1,275)	1:A:23:PHE:HA	1:A:27:LEU:H	9	0.24
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	8	0.24
(1,226)	1:A:49:VAL:HB	1:A:50:SER:H	12	0.24
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	1	0.24
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	12	0.24
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	1	0.24
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	2	0.24
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	4	0.24
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	9	0.24
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	13	0.24
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	16	0.24
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	1	0.24
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	10	0.24
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	13	0.24
(1,138)	1:A:13:ILE:HA	1:A:16:SER:H	3	0.24
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	2	0.24
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	2	0.24
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE1	12	0.24
(1,134)	1:A:56:VAL:H	1:A:57:TYR:HE2	12	0.24
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	1	0.23
(1,464)	1:A:45:ASN:HB2	1:A:46:ILE:H	4	0.23
(1,464)	1:A:45:ASN:HB3	1:A:46:ILE:H	4	0.23
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	4	0.23
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	4	0.23
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	15	0.23
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	15	0.23
(1,362)	1:A:53:LYS:H	1:A:53:LYS:HG3	10	0.23
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	7	0.23
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	7	0.23
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	2	0.23
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	15	0.23
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	7	0.23
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	5	0.23
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	6	0.23
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	14	0.23
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	14	0.23
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	14	0.23
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	16	0.23
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	16	0.23
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	2	0.22
(2,38)	1:C:30:THR:H	1:B:26:PHE:HB2	13	0.22
(2,38)	1:C:30:THR:H	1:D:26:PHE:HB2	13	0.22
(2,12)	1:B:16:SER:H	1:A:12:LEU:HD11	7	0.22
(2,12)	1:B:16:SER:H	1:A:12:LEU:HD12	7	0.22
(2,12)	1:B:16:SER:H	1:A:12:LEU:HD13	7	0.22
(2,12)	1:B:16:SER:H	1:C:12:LEU:HD11	7	0.22
(2,12)	1:B:16:SER:H	1:C:12:LEU:HD12	7	0.22
(2,12)	1:B:16:SER:H	1:C:12:LEU:HD13	7	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	9	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	9	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	9	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	9	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	9	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	9	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	10	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	10	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	10	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	10	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	10	0.22
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	10	0.22
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	16	0.22
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	16	0.22
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	16	0.22
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	16	0.22
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	16	0.22
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	16	0.22
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	2	0.22
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	2	0.22
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE1	9	0.22
(1,370)	1:A:26:PHE:H	1:A:26:PHE:HE2	9	0.22
(1,366)	1:A:53:LYS:H	1:A:53:LYS:HG2	16	0.22
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	13	0.22
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	14	0.22
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	4	0.22
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	7	0.22
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	11	0.22
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	15	0.22
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	2	0.22
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	6	0.22
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	15	0.22
(1,136)	1:A:55:THR:HB	1:A:56:VAL:H	3	0.22
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	8	0.21
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	7	0.21
(2,40)	1:E:30:THR:H	1:A:26:PHE:HB2	13	0.21
(2,40)	1:E:30:THR:H	1:D:26:PHE:HB2	13	0.21
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	8	0.21
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	8	0.21
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	10	0.21
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	12	0.21
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	12	0.21
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	14	0.21
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	14	0.21
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	15	0.21
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	15	0.21
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	12	0.21
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	12	0.21
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	14	0.21
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	14	0.21
(1,229)	1:A:50:SER:H	1:A:52:VAL:H	5	0.21
(1,218)	1:A:15:ASN:HA	1:A:15:ASN:HD22	3	0.21
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	16	0.21
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	13	0.21
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	16	0.21
(1,182)	1:A:56:VAL:HB	1:A:57:TYR:H	5	0.21
(1,153)	1:A:45:ASN:HA	1:A:45:ASN:HD22	3	0.21
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	12	0.21
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	3	0.21
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	3	0.21
(2,39)	1:D:30:THR:H	1:C:26:PHE:HB2	13	0.2
(2,39)	1:D:30:THR:H	1:E:26:PHE:HB2	13	0.2
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	13	0.2
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	13	0.2
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	16	0.2
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	16	0.2
(2,34)	1:D:30:THR:H	1:C:30:THR:HA	10	0.2
(2,34)	1:D:30:THR:H	1:E:30:THR:HA	10	0.2
(2,31)	1:A:30:THR:H	1:B:30:THR:HA	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:A:30:THR:H	1:E:30:THR:HA	6	0.2
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	4	0.2
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	4	0.2
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	16	0.2
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	16	0.2
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	16	0.2
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	16	0.2
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	16	0.2
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	16	0.2
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	13	0.2
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	13	0.2
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	5	0.2
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	5	0.2
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	9	0.2
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	9	0.2
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	2	0.2
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	7	0.2
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	10	0.2
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	11	0.2
(1,159)	1:A:49:VAL:H	1:A:51:LEU:H	13	0.2
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	14	0.2
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	14	0.2
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	14	0.2
(1,14)	1:A:30:THR:HB	1:A:31:LEU:H	4	0.2
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	2	0.2
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	2	0.2
(2,28)	1:C:28:LEU:H	1:B:24:VAL:HA	10	0.19
(2,28)	1:C:28:LEU:H	1:D:24:VAL:HA	10	0.19
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	7	0.19
(1,74)	1:A:33:ILE:HB	1:A:36:ALA:H	4	0.19
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	5	0.19
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	9	0.19
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	13	0.19
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	5	0.19
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	5	0.19
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	3	0.19
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	3	0.19
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	2	0.19
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	3	0.19
(1,337)	1:A:11:THR:HA	1:A:14:VAL:H	9	0.19
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	6	0.19
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	9	0.19
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	9	0.19
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE1	7	0.19
(1,316)	1:A:23:PHE:H	1:A:23:PHE:HE2	7	0.19
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	11	0.19
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	8	0.19
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	9	0.19
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	15	0.19
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	10	0.19
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	10	0.19
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	10	0.19
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	5	0.18
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	5	0.18
(2,36)	1:A:30:THR:H	1:B:26:PHE:HB2	3	0.18
(2,36)	1:A:30:THR:H	1:E:26:PHE:HB2	3	0.18
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	14	0.18
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	14	0.18
(1,98)	1:A:16:SER:H	1:A:18:LEU:H	9	0.18
(1,494)	1:A:62:VAL:HG11	1:A:65:LEU:H	16	0.18
(1,494)	1:A:62:VAL:HG12	1:A:65:LEU:H	16	0.18
(1,494)	1:A:62:VAL:HG13	1:A:65:LEU:H	16	0.18
(1,494)	1:A:62:VAL:HG21	1:A:65:LEU:H	16	0.18
(1,494)	1:A:62:VAL:HG22	1:A:65:LEU:H	16	0.18
(1,494)	1:A:62:VAL:HG23	1:A:65:LEU:H	16	0.18
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	3	0.18
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	3	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	14	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	14	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	14	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	14	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	14	0.18
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	14	0.18
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	12	0.18
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	12	0.18
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	12	0.18
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	12	0.18
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	12	0.18
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	12	0.18
(1,429)	1:A:23:PHE:HB2	1:A:24:VAL:H	2	0.18
(1,429)	1:A:23:PHE:HB3	1:A:24:VAL:H	2	0.18
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	10	0.18
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB1	2	0.18
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB2	2	0.18
(1,234)	1:A:30:THR:H	1:A:32:ALA:HB3	2	0.18
(1,136)	1:A:55:THR:HB	1:A:56:VAL:H	14	0.18
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	1	0.17
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	4	0.17
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD11	11	0.17
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD12	11	0.17
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD13	11	0.17
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD11	11	0.17
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD12	11	0.17
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD13	11	0.17
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	14	0.17
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	5	0.17
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	4	0.17
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	4	0.17
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	12	0.17
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	12	0.17
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	12	0.17
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	12	0.17
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	12	0.17
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	12	0.17
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	2	0.17
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	2	0.17
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	10	0.17
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	10	0.17
(1,343)	1:A:28:LEU:H	1:A:30:THR:H	6	0.17
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	8	0.17
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	8	0.17
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	1	0.17
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	3	0.17
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	10	0.17
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	1	0.17
(1,189)	1:A:64:ASN:H	1:A:64:ASN:HB3	13	0.17
(1,189)	1:A:64:ASN:H	1:A:64:ASN:HB3	14	0.17
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	8	0.17
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	8	0.17
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	8	0.17
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	12	0.17
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	12	0.17
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	12	0.17
(1,152)	1:A:30:THR:HA	1:A:34:LEU:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:A:55:THR:HB	1:A:56:VAL:H	6	0.17
(2,46)	1:A:47:VAL:H	1:E:64:ASN:H	1	0.16
(2,31)	1:A:30:THR:H	1:B:30:THR:HA	9	0.16
(2,31)	1:A:30:THR:H	1:E:30:THR:HA	9	0.16
(2,31)	1:A:30:THR:H	1:B:30:THR:HA	10	0.16
(2,31)	1:A:30:THR:H	1:E:30:THR:HA	10	0.16
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	9	0.16
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	9	0.16
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	9	0.16
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	9	0.16
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	9	0.16
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	9	0.16
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD11	14	0.16
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD12	14	0.16
(2,13)	1:C:16:SER:H	1:B:12:LEU:HD13	14	0.16
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD11	14	0.16
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD12	14	0.16
(2,13)	1:C:16:SER:H	1:D:12:LEU:HD13	14	0.16
(1,51)	1:A:56:VAL:HA	1:A:60:SER:H	6	0.16
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	13	0.16
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	13	0.16
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	14	0.16
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	14	0.16
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	16	0.16
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	15	0.16
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	11	0.16
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	16	0.16
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	5	0.16
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	11	0.16
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	15	0.16
(1,189)	1:A:64:ASN:H	1:A:64:ASN:HB3	3	0.16
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	2	0.16
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	2	0.16
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	2	0.16
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	4	0.16
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	4	0.16
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	4	0.16
(1,152)	1:A:30:THR:HA	1:A:34:LEU:H	2	0.16
(1,15)	1:A:21:LEU:HB2	1:A:22:ALA:H	16	0.16
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	9	0.16
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	9	0.16
(2,49)	1:D:47:VAL:H	1:C:64:ASN:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	3	0.15
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	3	0.15
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	2	0.15
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	6	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	3	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	3	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	3	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	3	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	3	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	3	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	11	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	11	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	11	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	11	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	11	0.15
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	11	0.15
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	4	0.15
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	4	0.15
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	4	0.15
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	4	0.15
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	4	0.15
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	4	0.15
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	6	0.15
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	6	0.15
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	11	0.15
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	11	0.15
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	12	0.15
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	12	0.15
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	15	0.15
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	15	0.15
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	4	0.15
(1,29)	1:A:13:ILE:HA	1:A:17:VAL:H	5	0.15
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	8	0.15
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	1	0.15
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	8	0.15
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	10	0.15
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	13	0.15
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	16	0.15
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	16	0.15
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	16	0.15
(1,152)	1:A:30:THR:HA	1:A:34:LEU:H	15	0.15
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	11	0.15
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	11	0.15
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	8	0.15
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	8	0.15
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	10	0.15
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	10	0.15
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB2	1	0.14
(2,41)	1:A:39:LEU:H	1:E:57:TYR:HB3	1	0.14
(2,38)	1:C:30:THR:H	1:B:26:PHE:HB2	3	0.14
(2,38)	1:C:30:THR:H	1:D:26:PHE:HB2	3	0.14
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	9	0.14
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	9	0.14
(2,32)	1:B:30:THR:H	1:A:30:THR:HA	6	0.14
(2,32)	1:B:30:THR:H	1:C:30:THR:HA	6	0.14
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	16	0.14
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB2	7	0.14
(1,505)	1:A:65:LEU:H	1:A:65:LEU:HB3	7	0.14
(1,464)	1:A:45:ASN:HB2	1:A:46:ILE:H	7	0.14
(1,464)	1:A:45:ASN:HB3	1:A:46:ILE:H	7	0.14
(1,376)	1:A:25:VAL:HB	1:A:26:PHE:H	11	0.14
(1,362)	1:A:53:LYS:H	1:A:53:LYS:HG3	16	0.14
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	7	0.14
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	10	0.14
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	12	0.14
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	13	0.14
(1,303)	1:A:43:ALA:HA	1:A:45:ASN:H	14	0.14
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	7	0.14
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	12	0.14
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	2	0.14
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	4	0.14
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	12	0.14
(1,19)	1:A:54:PRO:HB3	1:A:55:THR:H	5	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	1	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	1	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	1	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	3	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	3	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	3	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	6	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	6	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	6	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	9	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	9	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	15	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	15	0.14
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	15	0.14
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	11	0.14
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	11	0.14
(2,32)	1:B:30:THR:H	1:A:30:THR:HA	16	0.13
(2,32)	1:B:30:THR:H	1:C:30:THR:HA	16	0.13
(2,30)	1:E:28:LEU:H	1:A:24:VAL:HA	9	0.13
(2,30)	1:E:28:LEU:H	1:D:24:VAL:HA	9	0.13
(1,87)	1:A:23:PHE:HB2	1:A:24:VAL:H	6	0.13
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	16	0.13
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	16	0.13
(1,464)	1:A:45:ASN:HB2	1:A:46:ILE:H	8	0.13
(1,464)	1:A:45:ASN:HB3	1:A:46:ILE:H	8	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	5	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	5	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	5	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	5	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	5	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	5	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD11	7	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD12	7	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD13	7	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD21	7	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD22	7	0.13
(1,452)	1:A:34:LEU:H	1:A:34:LEU:HD23	7	0.13
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD11	5	0.13
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD12	5	0.13
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD13	5	0.13
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD21	5	0.13
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD22	5	0.13
(1,445)	1:A:30:THR:H	1:A:31:LEU:HD23	5	0.13
(1,439)	1:A:27:LEU:HB2	1:A:30:THR:H	8	0.13
(1,439)	1:A:27:LEU:HB3	1:A:30:THR:H	8	0.13
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	13	0.13
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	13	0.13
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	5	0.13
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	8	0.13
(1,327)	1:A:37:LEU:HB2	1:A:39:LEU:H	3	0.13
(1,327)	1:A:37:LEU:HB3	1:A:39:LEU:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	3	0.13
(1,230)	1:A:51:LEU:H	1:A:52:VAL:H	4	0.13
(1,205)	1:A:37:LEU:H	1:A:39:LEU:H	8	0.13
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	3	0.13
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	6	0.13
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	16	0.13
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	11	0.13
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	11	0.13
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	11	0.13
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	4	0.13
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	4	0.13
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	4	0.13
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	5	0.13
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	5	0.13
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	5	0.13
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	14	0.13
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	14	0.13
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	14	0.13
(2,48)	1:C:47:VAL:H	1:B:64:ASN:H	6	0.12
(2,40)	1:E:30:THR:H	1:A:26:PHE:HB2	6	0.12
(2,40)	1:E:30:THR:H	1:D:26:PHE:HB2	6	0.12
(2,36)	1:A:30:THR:H	1:B:26:PHE:HB2	6	0.12
(2,36)	1:A:30:THR:H	1:E:26:PHE:HB2	6	0.12
(2,34)	1:D:30:THR:H	1:C:30:THR:HA	4	0.12
(2,34)	1:D:30:THR:H	1:E:30:THR:HA	4	0.12
(2,34)	1:D:30:THR:H	1:C:30:THR:HA	5	0.12
(2,34)	1:D:30:THR:H	1:E:30:THR:HA	5	0.12
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD21	8	0.12
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD22	8	0.12
(2,20)	1:E:16:SER:H	1:A:12:LEU:HD23	8	0.12
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD21	8	0.12
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD22	8	0.12
(2,20)	1:E:16:SER:H	1:D:12:LEU:HD23	8	0.12
(1,74)	1:A:33:ILE:HB	1:A:36:ALA:H	2	0.12
(1,71)	1:A:45:ASN:HB3	1:A:46:ILE:H	3	0.12
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	5	0.12
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	5	0.12
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG2	9	0.12
(1,477)	1:A:53:LYS:H	1:A:53:LYS:HG3	9	0.12
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD21	2	0.12
(1,467)	1:A:48:ASN:H	1:A:48:ASN:HD22	2	0.12
(1,464)	1:A:45:ASN:HB2	1:A:46:ILE:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:A:45:ASN:HB3	1:A:46:ILE:H	15	0.12
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	16	0.12
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	16	0.12
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	14	0.12
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	14	0.12
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH11	1	0.12
(1,387)	1:A:61:ARG:H	1:A:61:ARG:HH12	1	0.12
(1,378)	1:A:22:ALA:HA	1:A:26:PHE:H	15	0.12
(1,376)	1:A:25:VAL:HB	1:A:26:PHE:H	5	0.12
(1,351)	1:A:61:ARG:HB3	1:A:62:VAL:H	5	0.12
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	1	0.12
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	11	0.12
(1,342)	1:A:13:ILE:HB	1:A:14:VAL:H	15	0.12
(1,263)	1:A:64:ASN:HD21	1:A:65:LEU:H	7	0.12
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	15	0.12
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	5	0.12
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	6	0.12
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	13	0.12
(1,252)	1:A:34:LEU:HB3	1:A:35:THR:H	14	0.12
(1,240)	1:A:30:THR:H	1:A:32:ALA:H	7	0.12
(1,230)	1:A:51:LEU:H	1:A:52:VAL:H	2	0.12
(1,189)	1:A:64:ASN:H	1:A:64:ASN:HB3	6	0.12
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG11	10	0.12
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG12	10	0.12
(1,155)	1:A:49:VAL:H	1:A:49:VAL:HG13	10	0.12
(1,142)	1:A:13:ILE:HG21	1:A:16:SER:H	8	0.12
(1,142)	1:A:13:ILE:HG22	1:A:16:SER:H	8	0.12
(1,142)	1:A:13:ILE:HG23	1:A:16:SER:H	8	0.12
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	4	0.12
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	4	0.12
(1,139)	1:A:16:SER:H	1:A:16:SER:HB2	13	0.12
(1,139)	1:A:16:SER:H	1:A:16:SER:HB3	13	0.12
(2,50)	1:E:47:VAL:H	1:D:64:ASN:H	12	0.11
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB2	5	0.11
(2,45)	1:E:39:LEU:H	1:D:57:TYR:HB3	5	0.11
(2,38)	1:C:30:THR:H	1:B:26:PHE:HB2	9	0.11
(2,38)	1:C:30:THR:H	1:D:26:PHE:HB2	9	0.11
(2,37)	1:B:30:THR:H	1:A:26:PHE:HB2	9	0.11
(2,37)	1:B:30:THR:H	1:C:26:PHE:HB2	9	0.11
(2,35)	1:E:30:THR:H	1:A:30:THR:HA	1	0.11
(2,35)	1:E:30:THR:H	1:D:30:THR:HA	1	0.11
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD21	16	0.11

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD22	16	0.11
(2,19)	1:D:16:SER:H	1:C:12:LEU:HD23	16	0.11
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD21	16	0.11
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD22	16	0.11
(2,19)	1:D:16:SER:H	1:E:12:LEU:HD23	16	0.11
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD21	7	0.11
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD22	7	0.11
(2,16)	1:A:16:SER:H	1:B:12:LEU:HD23	7	0.11
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD21	7	0.11
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD22	7	0.11
(2,16)	1:A:16:SER:H	1:E:12:LEU:HD23	7	0.11
(1,464)	1:A:45:ASN:HB2	1:A:46:ILE:H	1	0.11
(1,464)	1:A:45:ASN:HB3	1:A:46:ILE:H	1	0.11
(1,406)	1:A:12:LEU:HB2	1:A:13:ILE:H	15	0.11
(1,406)	1:A:12:LEU:HB3	1:A:13:ILE:H	15	0.11
(1,398)	1:A:26:PHE:HD1	1:A:29:VAL:H	7	0.11
(1,398)	1:A:26:PHE:HD2	1:A:29:VAL:H	7	0.11
(1,366)	1:A:53:LYS:H	1:A:53:LYS:HG2	11	0.11
(1,366)	1:A:53:LYS:H	1:A:53:LYS:HG2	14	0.11
(1,366)	1:A:53:LYS:H	1:A:53:LYS:HG2	15	0.11
(1,362)	1:A:53:LYS:H	1:A:53:LYS:HG3	11	0.11
(1,351)	1:A:61:ARG:HB3	1:A:62:VAL:H	9	0.11
(1,343)	1:A:28:LEU:H	1:A:30:THR:H	15	0.11
(1,275)	1:A:23:PHE:HA	1:A:27:LEU:H	4	0.11
(1,258)	1:A:11:THR:H	1:A:12:LEU:H	7	0.11
(1,213)	1:A:58:VAL:H	1:A:58:VAL:HB	3	0.11
(1,203)	1:A:25:VAL:H	1:A:25:VAL:HB	9	0.11
(1,189)	1:A:64:ASN:H	1:A:64:ASN:HB3	5	0.11
(1,189)	1:A:64:ASN:H	1:A:64:ASN:HB3	10	0.11
(1,156)	1:A:48:ASN:HB2	1:A:49:VAL:H	10	0.11
(1,138)	1:A:13:ILE:HA	1:A:16:SER:H	9	0.11

10 Dihedral-angle violation analysis ⓘ

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value