



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:12 PM BST

PDB ID : 1BVE  
Title : HIV-1 PROTEASE-DMP323 COMPLEX IN SOLUTION, NMR, 28 STRUCTURES  
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Deposited on : 1996-01-16

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

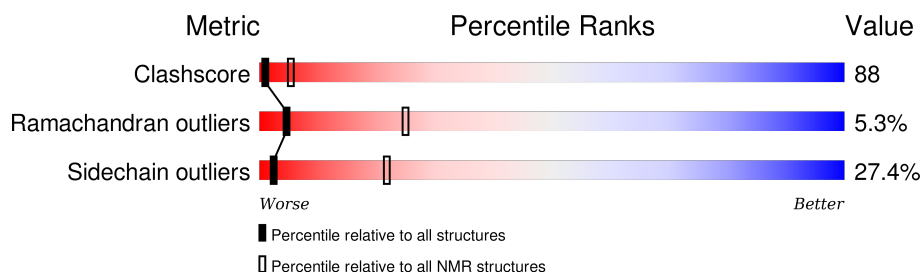
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	99	
1	B	99	

## 2 Ensemble composition and analysis

This entry contains 28 models. Model 7 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:1-A:99, B:1-B:99 (198)	0.54	7

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 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 9, 12, 14, 19, 22, 23, 27
2	7, 10, 15, 16, 18, 20, 24, 25, 26
3	4, 5, 6, 8, 21
4	2, 28
Single-model clusters	11; 13; 17

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3200 atoms, of which 1646 are hydrogens and 0 are deuteriums.

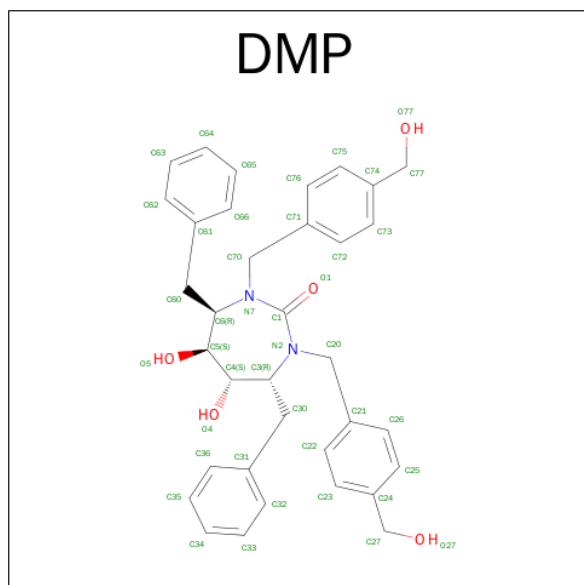
- Molecule 1 is a protein called HIV-1 PROTEASE.

Mol	Chain	Residues	Atoms					Trace
1	A	99	Total	C	H	N	O	S
			1560	488	804	130	135	3
1	B	99	Total	C	H	N	O	S
			1560	488	804	130	135	3

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ALA	CYS	ENGINEERED	UNP P04585
B	95	ALA	CYS	ENGINEERED	UNP P04585

- Molecule 2 is [4-R-(-4-ALPHA,5-ALPHA,6-BETA,7-BETA)]-HEXAHYDRO-5,6-BIS(HYDROXY)-[1,3-BIS([4-HYDROXYMETHYL-PHENYL]METHYL)-4,7-BIS(PHENYLMETHYL)]-2H-1,3-DIAZEPINONE (three-letter code: DMP) (formula: C<sub>35</sub>H<sub>38</sub>N<sub>2</sub>O<sub>5</sub>).

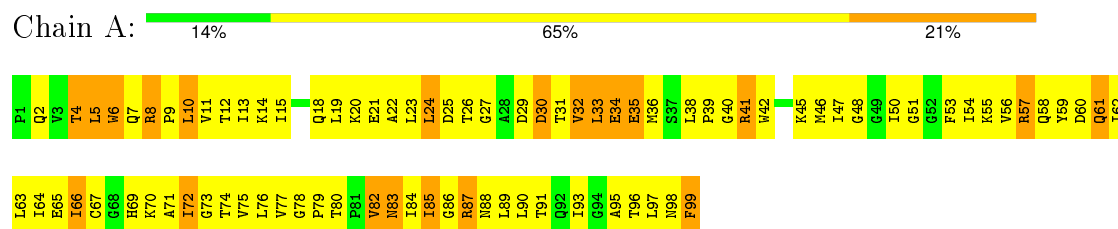


## 4 Residue-property plots

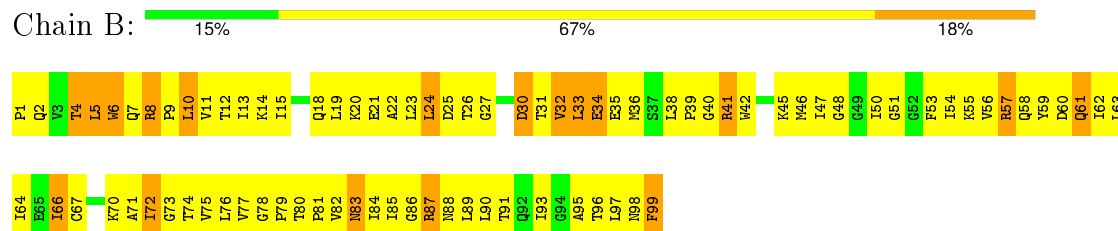
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: HIV-1 PROTEASE



#### • Molecule 1: HIV-1 PROTEASE

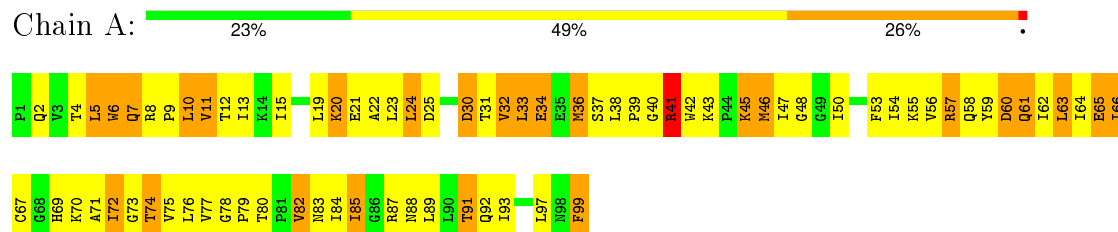


### 4.2 Scores per residue for each member of the ensemble

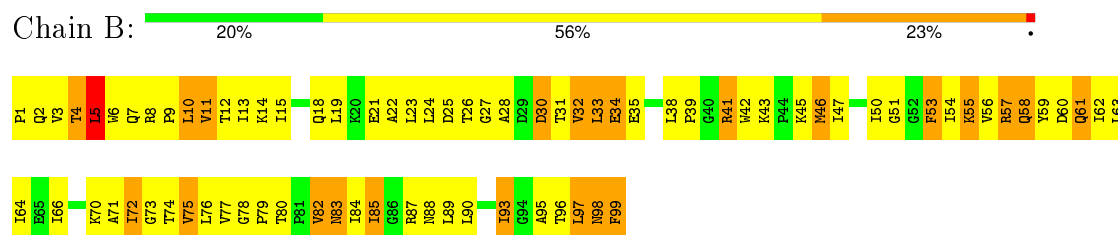
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

#### • Molecule 1: HIV-1 PROTEASE

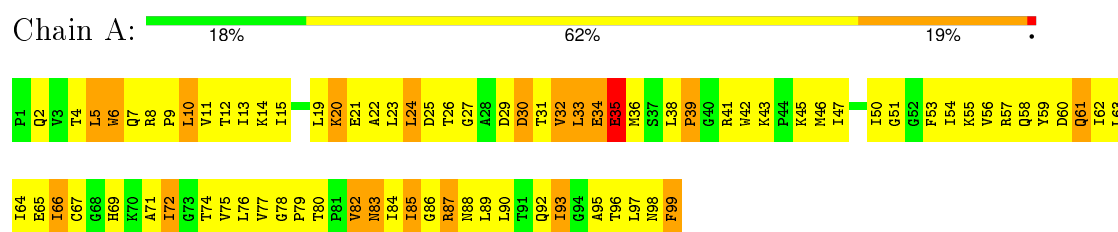


- Molecule 1: HIV-1 PROTEASE

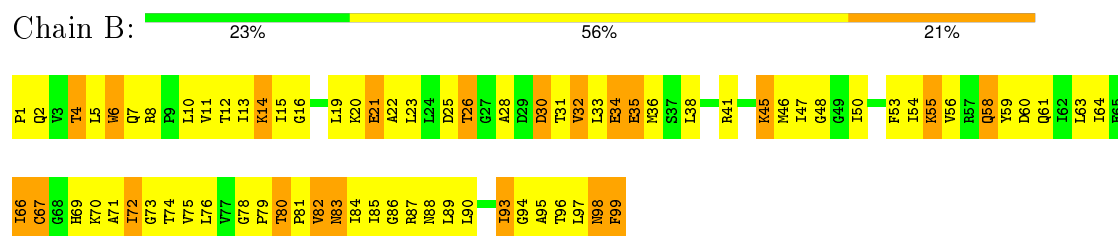


#### 4.2.2 Score per residue for model 2

- Molecule 1: HIV-1 PROTEASE

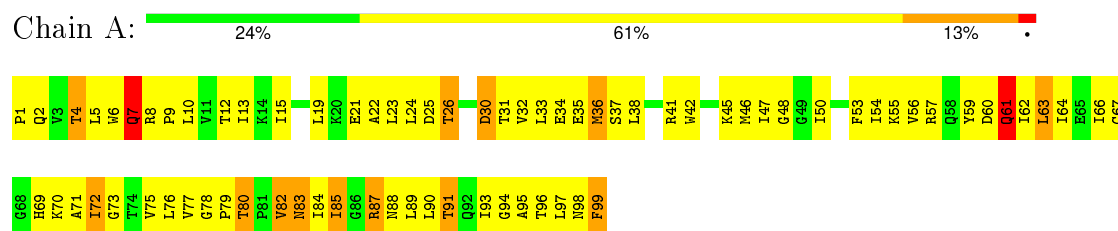


- Molecule 1: HIV-1 PROTEASE

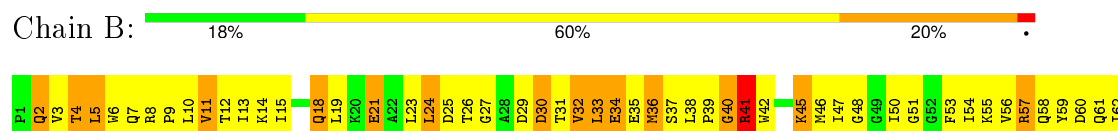


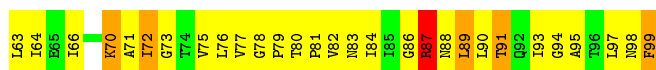
#### 4.2.3 Score per residue for model 3

- Molecule 1: HIV-1 PROTEASE



- Molecule 1: HIV-1 PROTEASE





#### 4.2.4 Score per residue for model 4

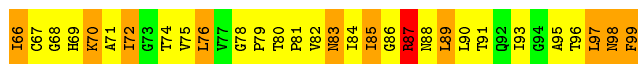
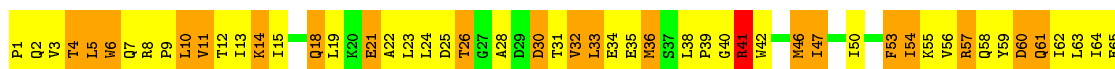
- Molecule 1: HIV-1 PROTEASE

Chain A: 19% 55% 25%



- Molecule 1: HIV-1 PROTEASE

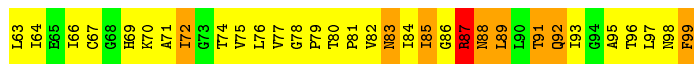
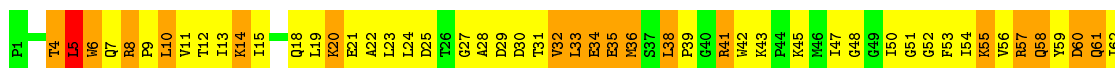
Chain B: 17% 51% 30%



#### 4.2.5 Score per residue for model 5

- Molecule 1: HIV-1 PROTEASE

Chain A: 16% 56% 26%



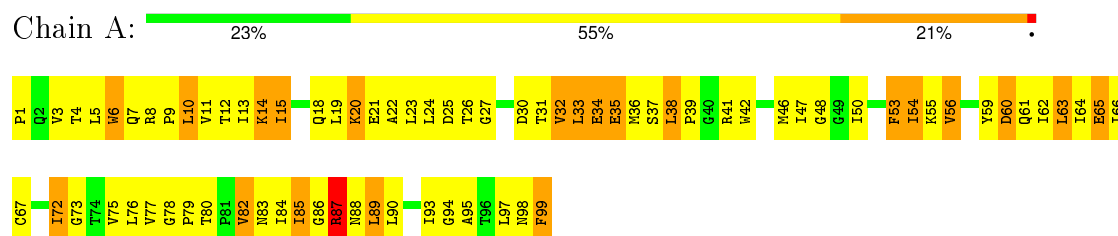
- Molecule 1: HIV-1 PROTEASE

Chain B: 20% 62% 16%

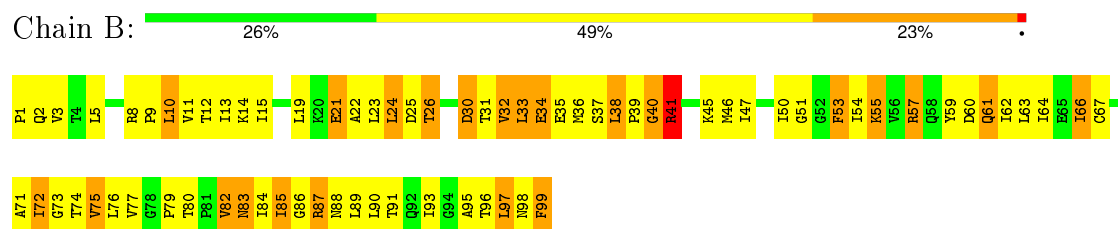


### 4.2.6 Score per residue for model 6

#### • Molecule 1: HIV-1 PROTEASE

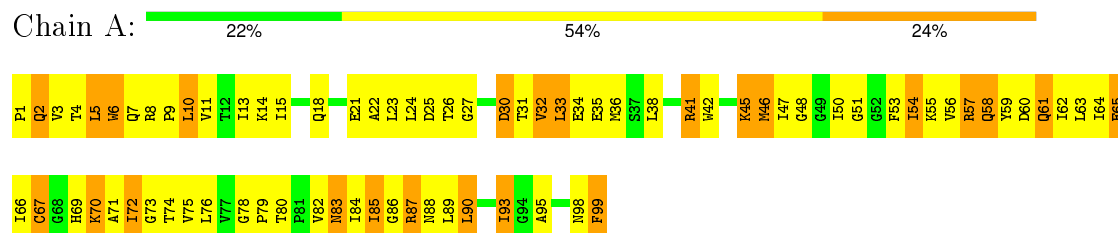


#### • Molecule 1: HIV-1 PROTEASE

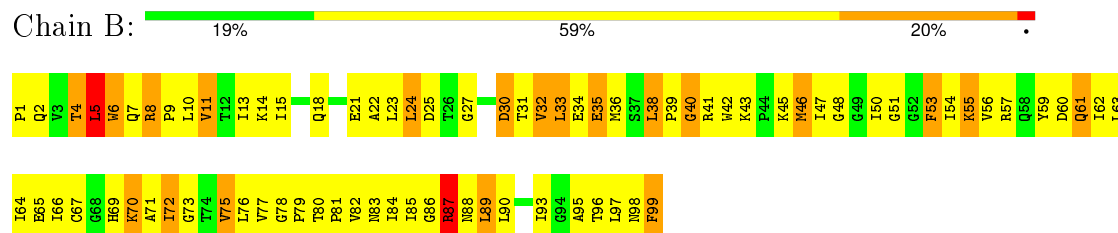


### 4.2.7 Score per residue for model 7 (medoid)

#### • Molecule 1: HIV-1 PROTEASE



#### • Molecule 1: HIV-1 PROTEASE

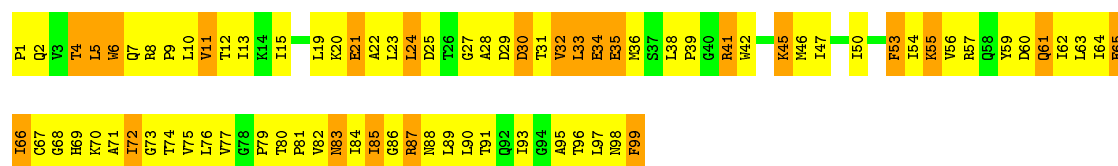


### 4.2.8 Score per residue for model 8

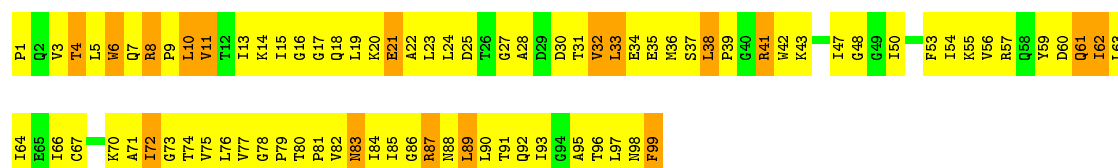
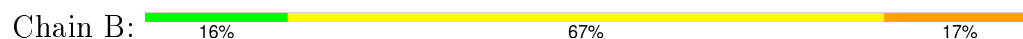
#### • Molecule 1: HIV-1 PROTEASE





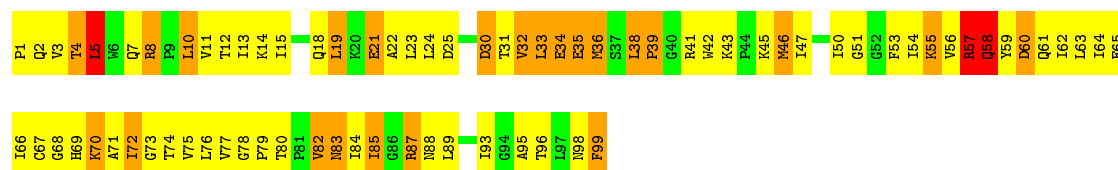


#### • Molecule 1: HIV-1 PROTEASE

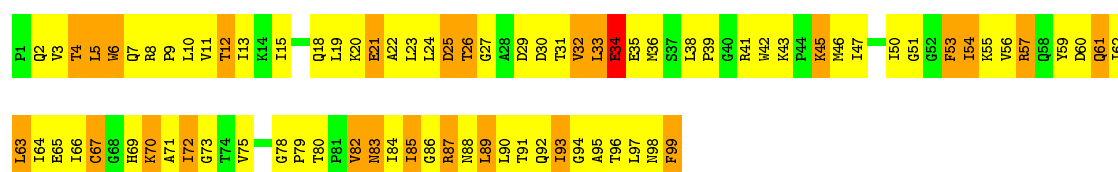
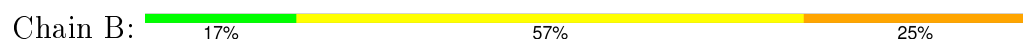


### 4.2.9 Score per residue for model 9

#### • Molecule 1: HIV-1 PROTEASE

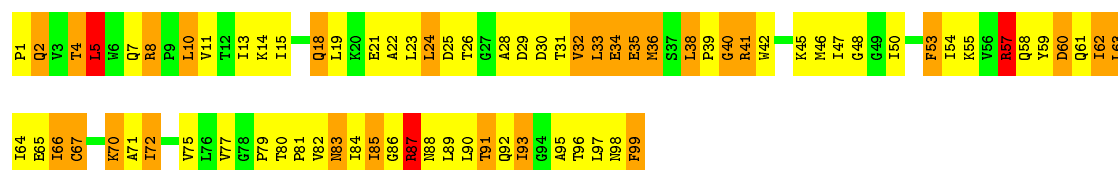


#### • Molecule 1: HIV-1 PROTEASE

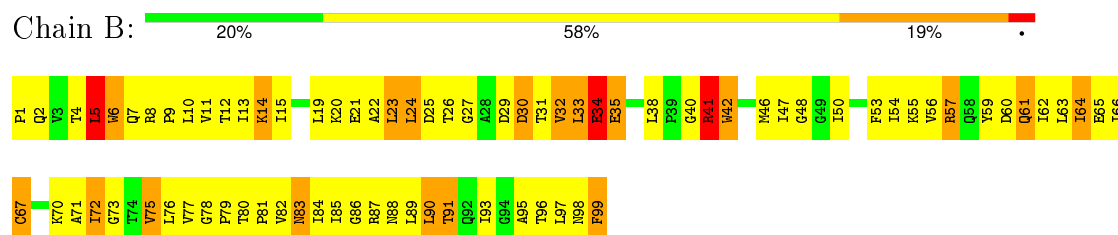


### 4.2.10 Score per residue for model 10

#### • Molecule 1: HIV-1 PROTEASE

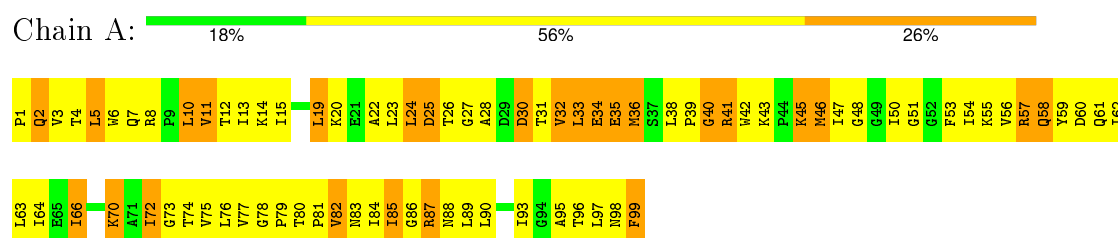


- Molecule 1: HIV-1 PROTEASE

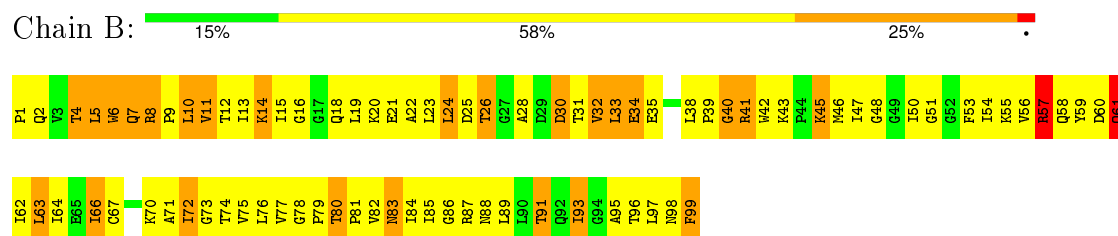


#### 4.2.11 Score per residue for model 11

- Molecule 1: HIV-1 PROTEASE

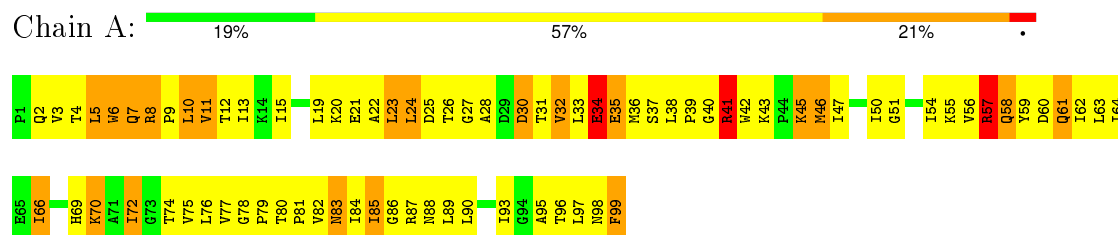


- Molecule 1: HIV-1 PROTEASE

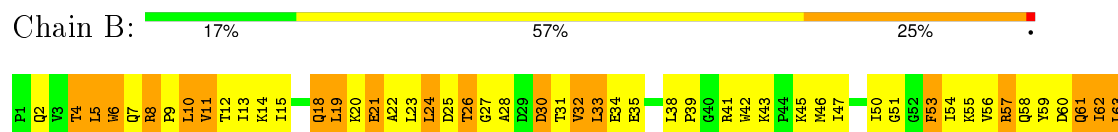


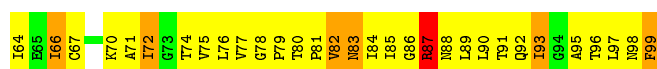
#### 4.2.12 Score per residue for model 12

- Molecule 1: HIV-1 PROTEASE



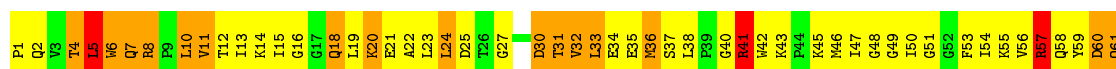
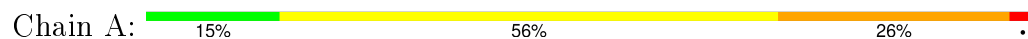
- Molecule 1: HIV-1 PROTEASE



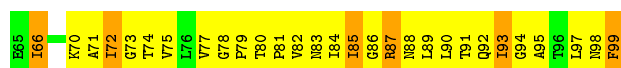
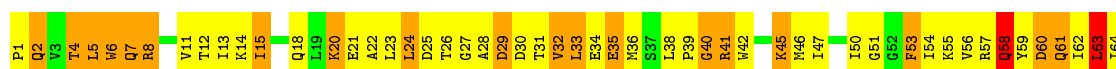


#### 4.2.13 Score per residue for model 13

- Molecule 1: HIV-1 PROTEASE

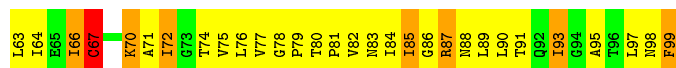
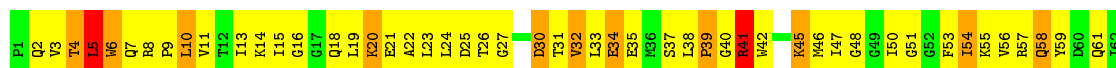
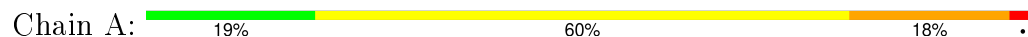


- Molecule 1: HIV-1 PROTEASE

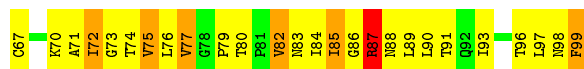


#### 4.2.14 Score per residue for model 14

- Molecule 1: HIV-1 PROTEASE

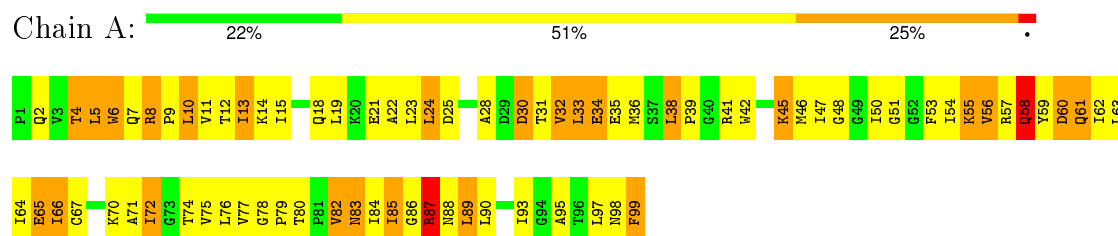


- Molecule 1: HIV-1 PROTEASE

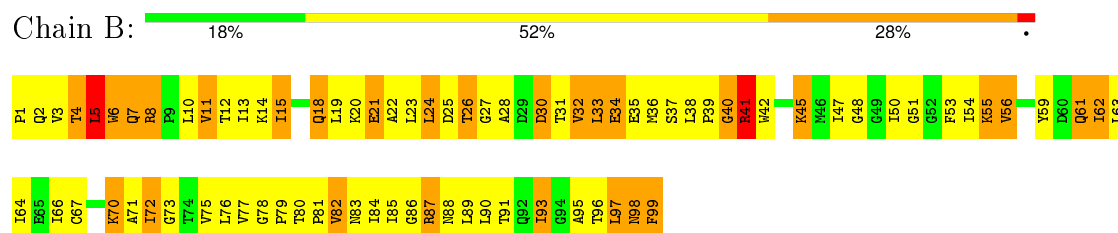


### 4.2.15 Score per residue for model 15

#### • Molecule 1: HIV-1 PROTEASE

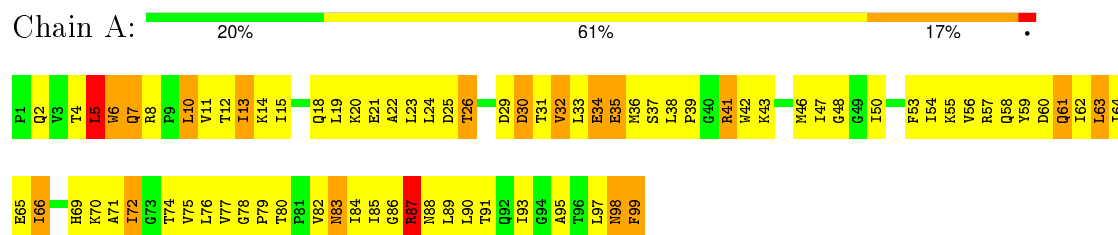


#### • Molecule 1: HIV-1 PROTEASE

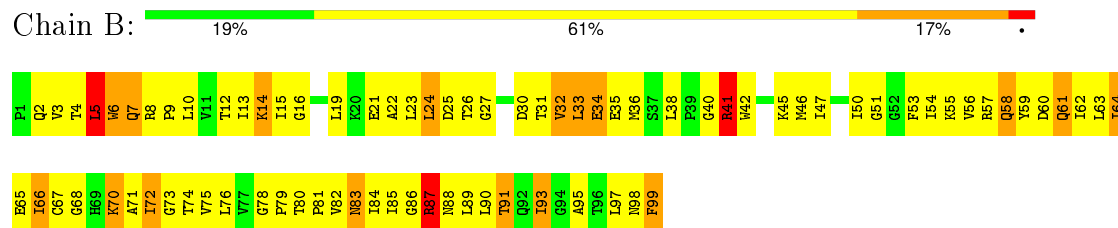


### 4.2.16 Score per residue for model 16

#### • Molecule 1: HIV-1 PROTEASE

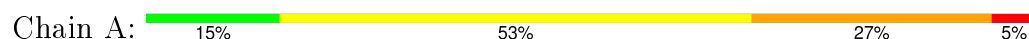


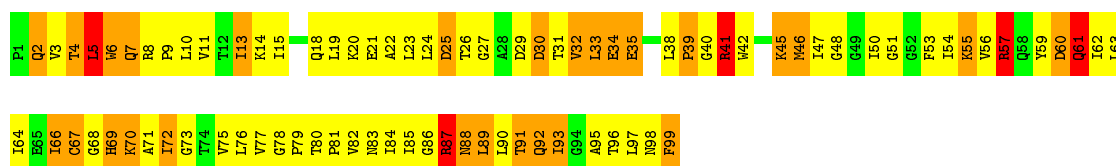
#### • Molecule 1: HIV-1 PROTEASE



### 4.2.17 Score per residue for model 17

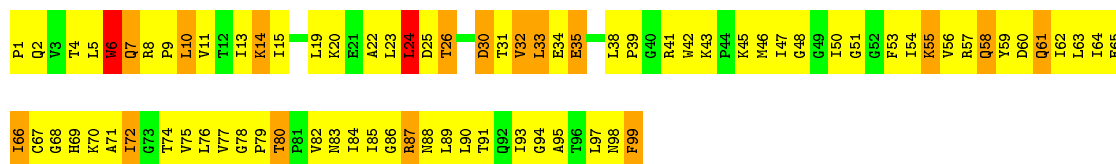
#### • Molecule 1: HIV-1 PROTEASE





#### • Molecule 1: HIV-1 PROTEASE

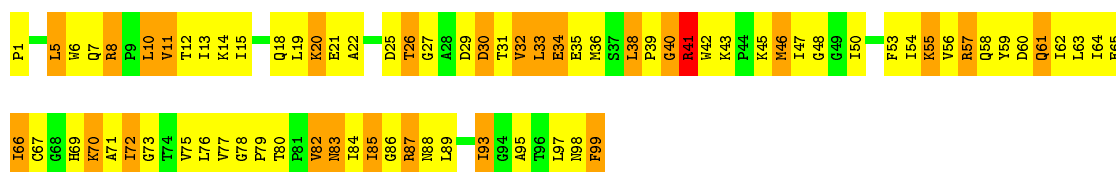
Chain B: 19% 63% 16%



### 4.2.18 Score per residue for model 18

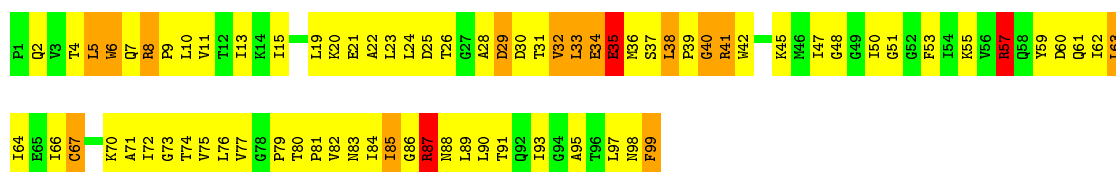
#### • Molecule 1: HIV-1 PROTEASE

Chain A: 22% 52% 25%



#### • Molecule 1: HIV-1 PROTEASE

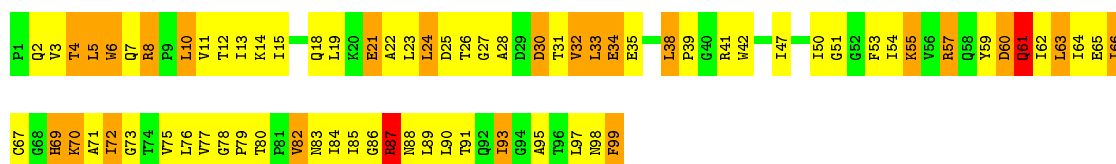
Chain B: 23% 60% 14%



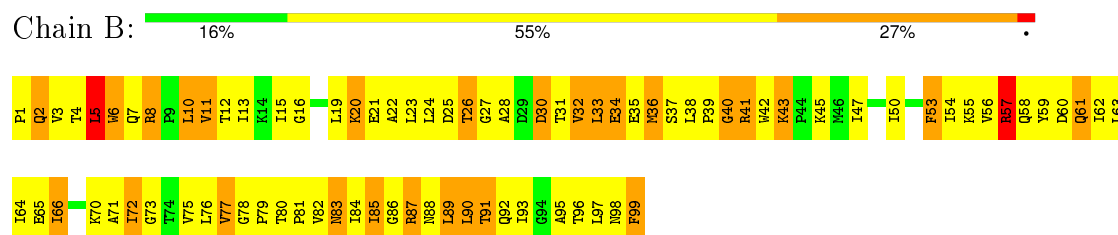
### 4.2.19 Score per residue for model 19

#### • Molecule 1: HIV-1 PROTEASE

Chain A: 24% 51% 23%

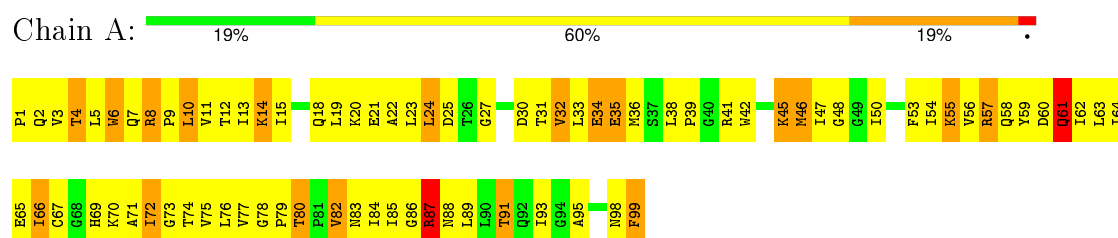


- Molecule 1: HIV-1 PROTEASE

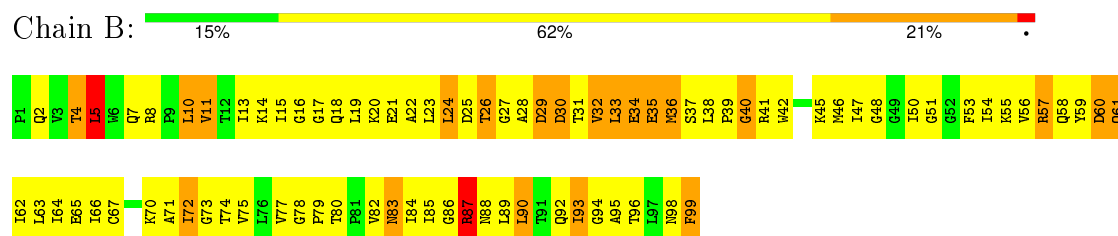


#### 4.2.20 Score per residue for model 20

- Molecule 1: HIV-1 PROTEASE

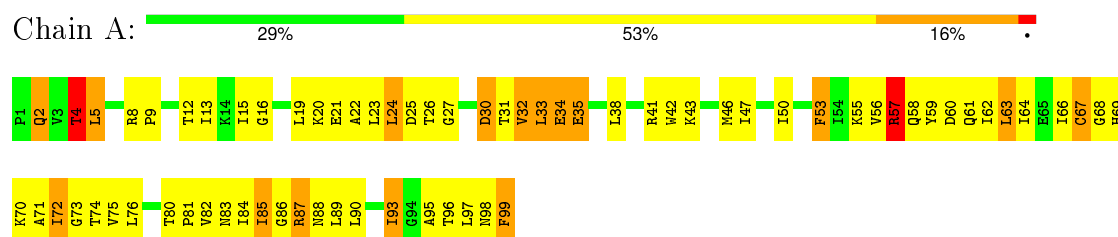


- Molecule 1: HIV-1 PROTEASE

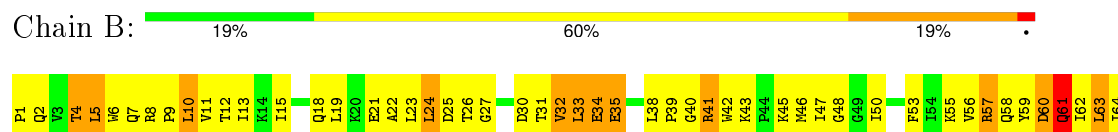


#### 4.2.21 Score per residue for model 21

- Molecule 1: HIV-1 PROTEASE



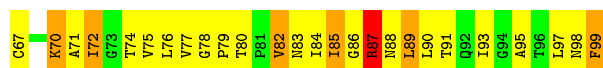
- Molecule 1: HIV-1 PROTEASE



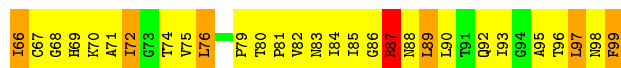


#### 4.2.22 Score per residue for model 22

##### • Molecule 1: HIV-1 PROTEASE



##### • Molecule 1: HIV-1 PROTEASE

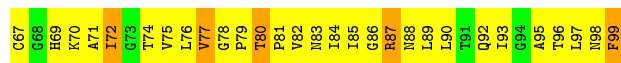
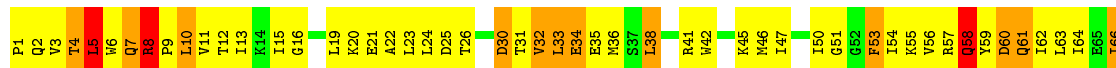
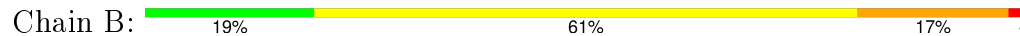


#### 4.2.23 Score per residue for model 23

##### • Molecule 1: HIV-1 PROTEASE

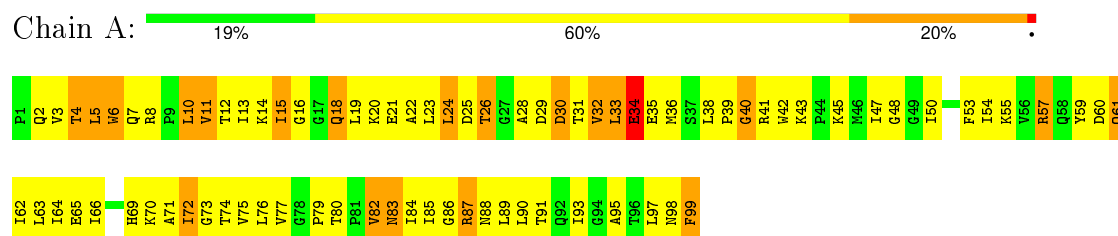


##### • Molecule 1: HIV-1 PROTEASE

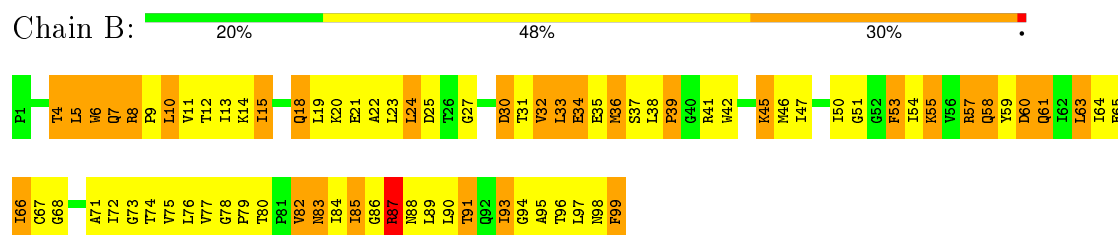


## 4.2.24 Score per residue for model 24

## • Molecule 1: HIV-1 PROTEASE

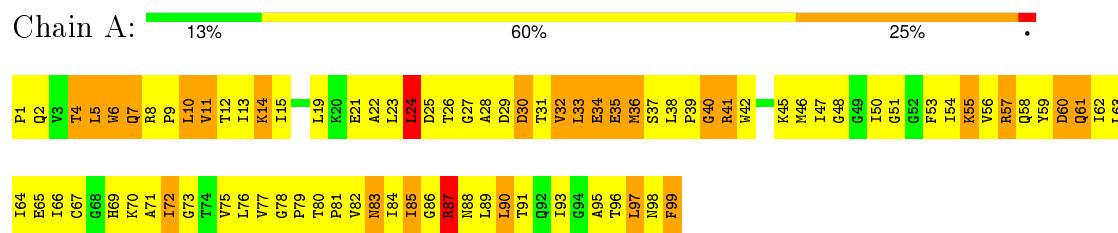


## • Molecule 1: HIV-1 PROTEASE

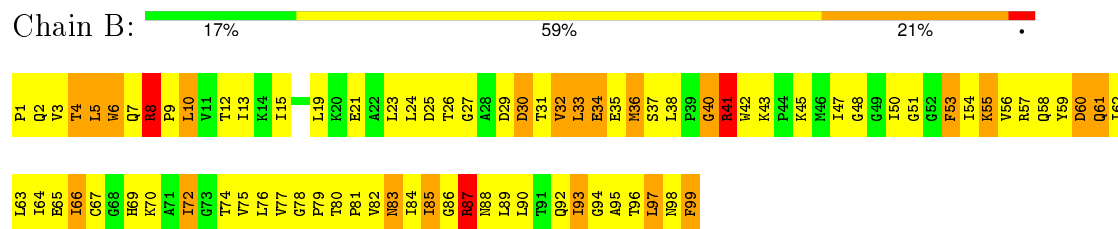


## 4.2.25 Score per residue for model 25

## • Molecule 1: HIV-1 PROTEASE

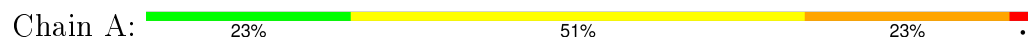


## • Molecule 1: HIV-1 PROTEASE

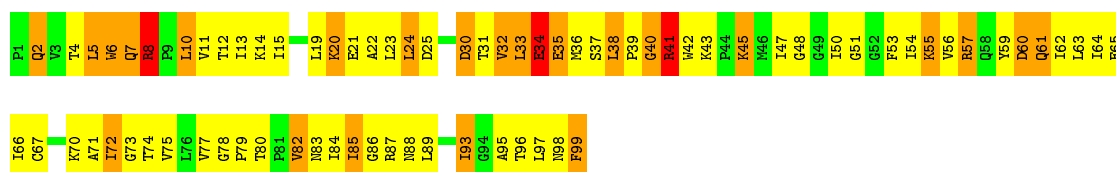


## 4.2.26 Score per residue for model 26

## • Molecule 1: HIV-1 PROTEASE

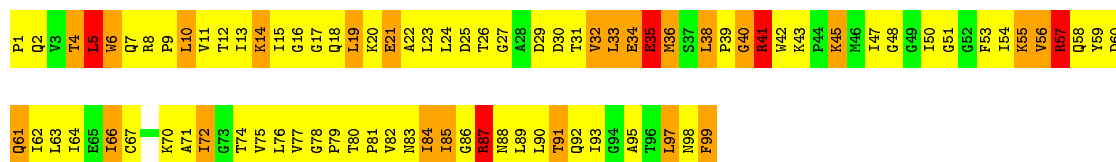






• Molecule 1: HIV-1 PROTEASE

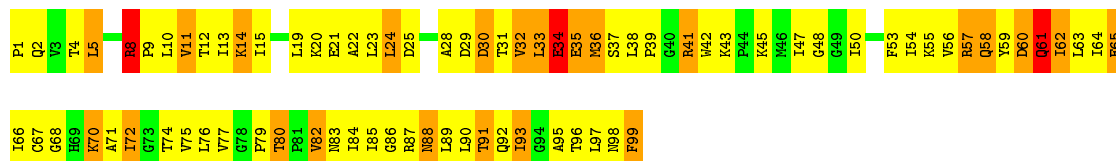
Chain B: 13% 59% 23% 5%



#### 4.2.27 Score per residue for model 27

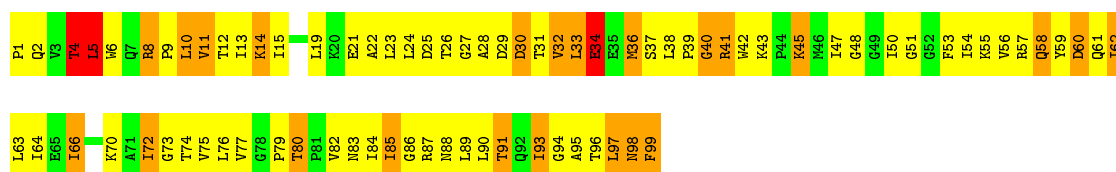
• Molecule 1: HIV-1 PROTEASE

Chain A: 19% 55% 23% .



• Molecule 1: HIV-1 PROTEASE

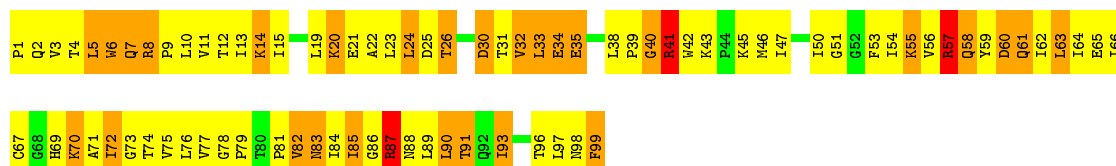
Chain B: 19% 55% 23% .



#### 4.2.28 Score per residue for model 28

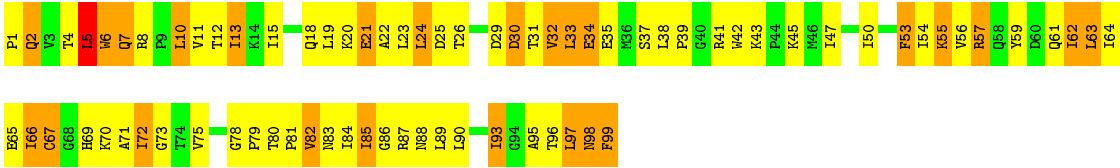
• Molecule 1: HIV-1 PROTEASE

Chain A: 17% 52% 28% .



● Molecule 1: HIV-1 PROTEASE

Chain B: 



## 5 Refinement protocol and experimental data overview

Of the 28 calculated structures, 28 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
XPLOR	structure solution	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMP

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.8±0.4
1	B	0.0±0.0	3.7±0.5
All	All	0	211

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	8	ARG	Sidechain	28
1	B	8	ARG	Sidechain	28
1	A	57	ARG	Sidechain	27
1	B	41	ARG	Sidechain	27
1	A	41	ARG	Sidechain	26
1	A	87	ARG	Sidechain	26
1	B	57	ARG	Sidechain	25
1	B	87	ARG	Sidechain	24

### 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	756	804	804	159±13
1	B	756	804	804	160±14
2	B	42	38	38	17±4
All	All	43512	46088	46088	7903

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 88.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HD13	1:A:92:GLN:OE1	1.05	1.52	17	2
1:A:63:LEU:HD21	1:A:70:LYS:CG	1.04	1.82	7	11
1:B:33:LEU:HD13	1:B:75:VAL:CG1	1.03	1.82	14	28
1:B:63:LEU:HD21	1:B:70:LYS:CG	1.03	1.82	27	9
1:A:33:LEU:HD13	1:A:75:VAL:CG1	1.01	1.86	24	28
1:B:22:ALA:HB1	1:B:85:ILE:HD13	1.00	1.32	24	9
1:B:15:ILE:HG23	1:B:62:ILE:CG2	0.98	1.88	18	17
1:A:93:ILE:HD12	1:B:99:PHE:CB	0.97	1.89	11	26
1:A:64:ILE:HD13	1:A:66:ILE:HD11	0.97	1.36	5	12
1:A:22:ALA:HB1	1:A:85:ILE:HD13	0.95	1.39	14	8
1:A:32:VAL:O	1:A:33:LEU:HD12	0.95	1.59	24	21
1:B:32:VAL:O	1:B:33:LEU:HD12	0.95	1.61	25	26
1:B:25:ASP:CB	1:B:84:ILE:HG23	0.95	1.91	28	23
1:B:88:ASN:ND2	1:B:89:LEU:HD23	0.95	1.77	26	27
1:A:88:ASN:ND2	1:A:89:LEU:HD23	0.95	1.76	10	27
1:A:13:ILE:HD11	1:A:33:LEU:HD21	0.94	1.37	11	14
1:A:27:GLY:O	1:B:23:LEU:HD21	0.94	1.63	2	15
1:B:13:ILE:O	1:B:19:LEU:HD23	0.94	1.62	25	16
1:A:12:THR:HG22	1:A:19:LEU:HD22	0.94	1.37	27	20
1:A:47:ILE:HD11	1:A:54:ILE:HD11	0.94	1.39	19	13
1:B:38:LEU:HD21	1:B:62:ILE:HD12	0.94	1.35	28	3
1:B:33:LEU:HD13	1:B:75:VAL:HG13	0.93	1.39	27	25
1:A:15:ILE:HD11	1:A:64:ILE:HD12	0.93	1.36	15	14
1:A:23:LEU:HD21	1:B:27:GLY:O	0.93	1.64	27	18
1:A:38:LEU:HD23	1:A:59:TYR:CD1	0.93	1.98	19	2
1:B:10:LEU:HD23	1:B:21:GLU:HB3	0.92	1.41	24	3
1:B:85:ILE:HG22	1:B:90:LEU:HD11	0.92	1.42	21	2
1:A:25:ASP:CB	1:A:84:ILE:HG23	0.92	1.94	15	17
1:B:11:VAL:HG22	1:B:22:ALA:HB3	0.92	1.42	14	4
1:A:3:VAL:HG13	1:A:5:LEU:HD23	0.92	1.39	24	1
1:B:63:LEU:O	1:B:63:LEU:HD13	0.91	1.65	28	12
1:A:5:LEU:O	1:A:5:LEU:HD22	0.91	1.62	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ILE:CG2	1:A:89:LEU:HD11	0.91	1.96	17	19
1:A:31:THR:O	1:A:76:LEU:HD12	0.91	1.65	16	1
1:A:26:THR:OG1	1:B:97:LEU:HD21	0.91	1.64	17	1
1:B:84:ILE:HD11	2:B:100:DMP:C32	0.91	1.96	17	9
1:B:45:LYS:NZ	1:B:76:LEU:HD23	0.91	1.80	26	2
1:A:63:LEU:HD21	1:A:70:LYS:HG2	0.90	1.44	7	8
1:A:99:PHE:CB	1:B:93:ILE:HD12	0.90	1.94	18	24
1:A:4:THR:HG21	1:B:96:THR:HG22	0.90	1.44	8	2
1:B:8:ARG:HD2	1:B:23:LEU:HD13	0.90	1.44	5	1
1:A:38:LEU:HD12	1:A:77:VAL:HG21	0.90	1.44	25	8
1:B:38:LEU:HD12	1:B:77:VAL:HG21	0.89	1.42	21	11
1:A:33:LEU:HD13	1:A:75:VAL:HG13	0.89	1.42	17	24
1:A:23:LEU:HD11	1:B:87:ARG:NH2	0.89	1.82	9	1
1:B:4:THR:O	1:B:5:LEU:HD22	0.89	1.68	26	1
1:B:5:LEU:N	1:B:5:LEU:HD13	0.89	1.82	26	1
1:A:14:LYS:HD3	1:A:19:LEU:HD21	0.88	1.45	20	3
1:B:15:ILE:HD13	1:B:75:VAL:HG11	0.88	1.45	19	23
1:B:13:ILE:HG22	1:B:66:ILE:HG13	0.88	1.43	24	22
1:B:15:ILE:HG23	1:B:62:ILE:HG21	0.88	1.46	18	15
1:A:4:THR:CG2	1:B:96:THR:HG22	0.88	1.98	8	13
1:B:4:THR:C	1:B:5:LEU:HD22	0.88	1.89	26	1
1:A:63:LEU:HD13	1:A:64:ILE:N	0.87	1.83	14	1
1:A:15:ILE:HG23	1:A:62:ILE:CG2	0.87	1.99	18	13
1:A:63:LEU:HD11	1:A:70:LYS:HG2	0.87	1.46	27	2
1:B:10:LEU:HD22	1:B:21:GLU:HB3	0.87	1.44	4	8
1:B:85:ILE:HG22	1:B:90:LEU:CD1	0.87	2.00	21	2
1:B:12:THR:HG22	1:B:19:LEU:HD22	0.87	1.44	24	17
1:B:63:LEU:HD21	1:B:70:LYS:HG2	0.87	1.45	3	8
1:A:93:ILE:HD12	1:B:99:PHE:CG	0.86	2.05	19	27
1:B:11:VAL:HG21	1:B:66:ILE:HG23	0.86	1.48	7	6
1:A:63:LEU:HD13	1:A:63:LEU:O	0.86	1.71	18	9
1:A:75:VAL:C	1:A:76:LEU:HD12	0.86	1.90	20	1
1:B:22:ALA:HB1	1:B:85:ILE:CD1	0.86	2.01	12	19
1:B:13:ILE:CD1	1:B:15:ILE:HD12	0.86	2.01	13	7
1:B:62:ILE:HD13	1:B:75:VAL:HG23	0.86	1.45	17	3
1:B:63:LEU:HD21	1:B:70:LYS:HG3	0.86	1.47	27	8
1:A:10:LEU:HD23	1:A:21:GLU:HB3	0.86	1.47	5	4
1:A:5:LEU:HD22	1:A:5:LEU:O	0.86	1.67	9	1
1:B:13:ILE:HD13	1:B:15:ILE:HD12	0.86	1.46	13	2
1:B:45:LYS:CE	1:B:56:VAL:HG23	0.86	2.00	26	2
1:B:59:TYR:HB3	1:B:62:ILE:HD11	0.86	1.47	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:CD1	1:A:75:VAL:HG21	0.85	2.01	6	2
1:B:4:THR:C	1:B:5:LEU:HD13	0.85	1.92	27	2
1:A:50:ILE:HD12	2:B:100:DMP:H702	0.85	1.46	3	24
1:A:15:ILE:HD13	1:A:75:VAL:HG11	0.85	1.46	1	21
1:A:11:VAL:HG22	1:A:22:ALA:HB3	0.85	1.46	27	4
1:A:26:THR:HG21	1:A:97:LEU:HD22	0.84	1.49	14	1
1:A:97:LEU:HD11	1:B:97:LEU:HD11	0.84	1.48	1	24
1:A:84:ILE:HD11	2:B:100:DMP:C62	0.84	2.03	12	1
1:B:60:ASP:OD1	1:B:74:THR:HG23	0.83	1.73	17	4
1:B:64:ILE:CG2	1:B:89:LEU:HD11	0.83	2.04	9	18
1:A:22:ALA:HB1	1:A:85:ILE:CD1	0.83	2.02	12	16
1:A:63:LEU:O	1:A:63:LEU:HD13	0.83	1.73	1	5
1:B:9:PRO:HB2	1:B:24:LEU:HD12	0.83	1.50	12	12
1:A:64:ILE:CD1	1:A:66:ILE:HD11	0.83	2.03	4	12
1:A:11:VAL:HG21	1:A:66:ILE:HG23	0.83	1.50	4	8
1:A:50:ILE:HG21	1:B:47:ILE:HD12	0.83	1.48	2	15
1:B:31:THR:HG23	1:B:85:ILE:HD12	0.83	1.51	5	8
1:A:93:ILE:HD12	1:B:99:PHE:HB2	0.82	1.50	11	6
1:B:15:ILE:HG22	1:B:38:LEU:HD21	0.82	1.51	25	3
1:A:97:LEU:HD13	1:B:97:LEU:HD13	0.82	1.50	25	1
1:A:13:ILE:O	1:A:19:LEU:HD23	0.82	1.74	1	18
1:A:63:LEU:HD21	1:A:70:LYS:HG3	0.82	1.51	7	9
1:B:63:LEU:HD13	1:B:63:LEU:O	0.82	1.74	2	5
1:B:50:ILE:HD12	2:B:100:DMP:C20	0.82	2.05	19	22
1:B:4:THR:O	1:B:5:LEU:HD12	0.82	1.73	5	1
1:B:56:VAL:HG12	1:B:78:GLY:HA3	0.82	1.52	5	15
1:A:45:LYS:O	1:A:56:VAL:HG22	0.82	1.75	26	3
1:B:11:VAL:HG23	1:B:13:ILE:HG23	0.82	1.52	26	5
1:A:30:ASP:HB3	1:A:76:LEU:HD11	0.81	1.50	12	9
1:A:26:THR:HG23	1:A:90:LEU:HD13	0.81	1.51	16	7
1:A:50:ILE:HD12	2:B:100:DMP:C70	0.81	2.05	13	27
1:B:36:MET:SD	1:B:38:LEU:HD22	0.81	2.14	18	2
1:B:25:ASP:HB3	1:B:84:ILE:HG23	0.81	1.50	7	14
1:A:96:THR:HG22	1:B:4:THR:HG22	0.81	1.51	17	4
1:A:56:VAL:HG12	1:A:78:GLY:HA3	0.81	1.50	13	16
1:B:50:ILE:HD12	2:B:100:DMP:H202	0.80	1.53	4	21
1:A:5:LEU:HD12	1:A:7:GLN:HB2	0.80	1.53	7	2
1:B:73:GLY:HA3	1:B:89:LEU:HD21	0.80	1.53	15	16
1:A:15:ILE:HD12	1:A:75:VAL:HG11	0.80	1.52	6	2
1:A:85:ILE:N	1:A:85:ILE:HD13	0.80	1.90	8	5
1:B:25:ASP:HB2	1:B:84:ILE:HG23	0.80	1.52	28	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:SER:O	1:A:38:LEU:HD22	0.80	1.76	1	1
1:B:45:LYS:CE	1:B:76:LEU:HD23	0.79	2.06	26	2
1:A:15:ILE:HG23	1:A:62:ILE:HG21	0.79	1.53	18	14
1:A:15:ILE:CD1	1:A:75:VAL:HG11	0.79	2.07	23	12
1:B:64:ILE:HD13	1:B:66:ILE:HD11	0.79	1.53	1	7
1:B:26:THR:HG23	1:B:90:LEU:HD23	0.79	1.54	14	2
1:A:99:PHE:CG	1:B:93:ILE:HD12	0.79	2.12	18	23
1:B:50:ILE:HD12	2:B:100:DMP:C21	0.79	2.08	8	21
1:B:30:ASP:HB3	1:B:76:LEU:HD11	0.79	1.53	17	10
1:A:50:ILE:HD12	2:B:100:DMP:C76	0.78	2.08	2	26
1:A:25:ASP:HB3	1:A:84:ILE:HG23	0.78	1.54	15	2
1:B:11:VAL:CG2	1:B:22:ALA:HB3	0.78	2.08	14	2
1:A:35:GLU:HA	1:A:77:VAL:HG12	0.78	1.55	10	10
1:B:38:LEU:HD12	1:B:39:PRO:CD	0.78	2.09	18	3
1:B:32:VAL:HG13	1:B:80:THR:HG21	0.78	1.55	13	14
1:A:33:LEU:HD13	1:A:75:VAL:HG12	0.77	1.56	23	9
1:B:90:LEU:O	1:B:95:ALA:HB3	0.77	1.79	13	4
1:A:32:VAL:HG13	1:A:80:THR:HG21	0.77	1.54	3	14
1:B:63:LEU:N	1:B:72:ILE:HD13	0.77	1.94	28	16
1:A:9:PRO:HB2	1:A:24:LEU:HD12	0.77	1.55	1	10
1:A:31:THR:HG23	1:A:84:ILE:O	0.77	1.79	20	9
1:A:85:ILE:HD13	1:A:85:ILE:N	0.77	1.92	3	3
1:B:59:TYR:CB	1:B:62:ILE:HD11	0.77	2.08	9	4
1:B:12:THR:CG2	1:B:19:LEU:HD22	0.76	2.08	27	6
1:A:5:LEU:HD23	1:B:91:THR:HG23	0.76	1.57	21	1
1:A:38:LEU:HD23	1:A:59:TYR:CD2	0.76	2.16	22	8
1:A:60:ASP:OD1	1:A:74:THR:HG23	0.76	1.81	15	7
1:A:64:ILE:HG21	1:A:89:LEU:HD11	0.76	1.57	17	3
1:A:64:ILE:HG22	1:A:71:ALA:O	0.76	1.81	14	15
1:A:25:ASP:HB2	1:A:84:ILE:HG23	0.75	1.57	20	12
1:B:69:HIS:HB2	1:B:93:ILE:HG22	0.75	1.57	25	1
1:A:31:THR:HG22	1:A:33:LEU:CD1	0.75	2.12	5	17
1:B:45:LYS:O	1:B:56:VAL:HG22	0.75	1.81	2	7
1:B:10:LEU:HD23	1:B:21:GLU:CB	0.75	2.11	24	1
1:B:11:VAL:HG23	1:B:13:ILE:CG2	0.75	2.12	26	4
1:A:38:LEU:CD1	1:A:77:VAL:HG21	0.75	2.11	24	3
1:A:47:ILE:CD1	1:B:50:ILE:HG21	0.75	2.11	25	17
1:A:95:ALA:HB3	1:B:5:LEU:HD12	0.75	1.57	6	1
1:A:59:TYR:HB3	1:A:62:ILE:HD11	0.75	1.59	1	6
1:A:93:ILE:HD12	1:B:99:PHE:HB3	0.75	1.57	24	12
1:B:62:ILE:HG21	1:B:75:VAL:HG21	0.75	1.59	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:13:ILE:HD11	1:B:33:LEU:HD21	0.75	1.58	18	9
1:B:89:LEU:HD13	1:B:92:GLN:OE1	0.75	1.82	21	2
1:B:15:ILE:CG2	1:B:38:LEU:HD21	0.74	2.12	25	6
1:A:32:VAL:HG12	1:A:84:ILE:CG1	0.74	2.12	1	21
1:A:73:GLY:HA3	1:A:89:LEU:HD21	0.74	1.57	19	13
1:A:99:PHE:HB3	1:B:93:ILE:HD12	0.74	1.57	15	10
1:A:85:ILE:HG22	1:A:90:LEU:HD11	0.74	1.60	25	1
1:A:5:LEU:HD13	1:A:5:LEU:C	0.74	2.03	18	1
1:A:50:ILE:HD12	2:B:100:DMP:C71	0.74	2.12	12	24
1:A:13:ILE:HG22	1:A:66:ILE:HG13	0.74	1.60	14	17
1:A:62:ILE:C	1:A:72:ILE:HD13	0.74	2.02	25	10
1:B:15:ILE:HD13	1:B:75:VAL:HG21	0.74	1.59	18	2
1:A:47:ILE:HD11	1:B:50:ILE:HG21	0.74	1.59	28	9
1:A:32:VAL:HG21	1:A:47:ILE:HD13	0.73	1.59	22	7
1:A:50:ILE:HG21	1:B:47:ILE:HD11	0.73	1.59	19	10
1:B:15:ILE:HD11	1:B:64:ILE:HD12	0.73	1.59	25	9
1:B:50:ILE:HD12	2:B:100:DMP:C26	0.73	2.13	10	22
1:B:10:LEU:HD22	1:B:21:GLU:HB2	0.73	1.60	8	1
1:A:99:PHE:CD2	1:B:93:ILE:HD12	0.73	2.19	23	16
1:B:38:LEU:HD12	1:B:77:VAL:CG2	0.73	2.14	21	9
1:A:58:GLN:OE1	1:A:74:THR:HG22	0.73	1.83	22	1
1:A:15:ILE:HD12	1:A:33:LEU:HD22	0.72	1.60	20	5
1:A:12:THR:CG2	1:A:19:LEU:HD22	0.72	2.14	27	10
1:A:50:ILE:HG21	1:B:47:ILE:CD1	0.72	2.15	15	17
1:A:90:LEU:O	1:A:95:ALA:HB3	0.72	1.84	13	4
1:A:32:VAL:HG23	1:A:76:LEU:HB2	0.72	1.61	12	8
1:A:5:LEU:HD23	1:B:87:ARG:HD2	0.72	1.60	18	1
1:A:66:ILE:HD11	1:A:89:LEU:CD1	0.72	2.14	17	1
1:B:38:LEU:HD12	1:B:59:TYR:CD2	0.72	2.19	15	1
1:A:50:ILE:HD11	1:B:84:ILE:CD1	0.72	2.15	15	1
1:A:26:THR:HG21	1:A:97:LEU:CD2	0.72	2.14	14	1
1:B:10:LEU:HD22	1:B:21:GLU:CB	0.72	2.14	4	5
1:B:32:VAL:HG12	1:B:84:ILE:CG1	0.72	2.15	14	10
1:B:31:THR:HG22	1:B:33:LEU:CD1	0.72	2.14	8	20
1:A:64:ILE:HG12	1:A:66:ILE:HD12	0.72	1.62	2	4
1:A:54:ILE:HD12	1:A:54:ILE:C	0.71	2.05	11	1
1:A:96:THR:HG22	1:B:4:THR:CG2	0.71	2.15	13	12
1:B:32:VAL:HG12	1:B:84:ILE:HB	0.71	1.60	4	10
1:A:12:THR:HG22	1:A:19:LEU:HD23	0.71	1.63	23	1
1:A:50:ILE:HG23	1:B:54:ILE:HD13	0.71	1.63	13	8
1:A:87:ARG:O	1:A:91:THR:HG23	0.71	1.85	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:45:LYS:HE3	1:B:76:LEU:HD23	0.71	1.62	15	2
1:A:99:PHE:HB2	1:B:93:ILE:HD12	0.70	1.63	18	4
1:B:42:TRP:CD1	1:B:59:TYR:CE1	0.70	2.79	12	7
1:B:10:LEU:HD23	1:B:22:ALA:C	0.70	2.05	22	3
1:B:38:LEU:HD21	1:B:62:ILE:CD1	0.70	2.15	28	4
1:B:15:ILE:CD1	1:B:75:VAL:HG11	0.70	2.16	18	13
1:A:63:LEU:HD13	1:A:63:LEU:C	0.70	2.07	14	7
1:A:47:ILE:CD1	1:A:54:ILE:HD11	0.70	2.16	19	2
1:A:34:GLU:HA	1:A:80:THR:HG22	0.70	1.62	12	12
1:B:88:ASN:HD21	1:B:89:LEU:HD23	0.70	1.44	21	13
1:B:62:ILE:C	1:B:72:ILE:HD13	0.70	2.06	12	14
1:A:38:LEU:HD23	1:A:59:TYR:CG	0.70	2.21	5	5
1:A:38:LEU:HD21	1:A:62:ILE:HD12	0.70	1.62	27	3
1:B:47:ILE:HD11	1:B:54:ILE:HD11	0.70	1.62	10	18
1:B:59:TYR:O	1:B:74:THR:HG23	0.70	1.85	2	2
1:B:24:LEU:CD2	1:B:85:ILE:HG21	0.70	2.17	27	5
1:A:24:LEU:CD2	1:A:90:LEU:HD21	0.70	2.15	4	1
1:A:13:ILE:CD1	1:A:33:LEU:HD21	0.70	2.16	11	7
1:A:38:LEU:HD11	1:A:62:ILE:HD12	0.70	1.64	7	2
1:A:10:LEU:HD23	1:A:21:GLU:CB	0.70	2.17	5	4
1:A:14:LYS:CD	1:A:19:LEU:HD21	0.70	2.16	25	5
1:B:15:ILE:HD12	1:B:33:LEU:CD2	0.70	2.17	17	10
1:B:15:ILE:CG2	1:B:62:ILE:CG2	0.70	2.70	15	3
1:B:26:THR:HG23	1:B:90:LEU:HD13	0.70	1.64	9	5
1:A:54:ILE:CD1	1:A:56:VAL:HG13	0.70	2.15	23	4
1:A:93:ILE:HD12	1:B:99:PHE:CD2	0.69	2.22	12	9
1:A:4:THR:C	1:A:5:LEU:HD12	0.69	2.08	9	1
1:B:64:ILE:HG12	1:B:66:ILE:HD12	0.69	1.65	23	6
1:B:24:LEU:HD22	1:B:90:LEU:HD21	0.69	1.62	6	8
1:A:11:VAL:HG23	1:A:13:ILE:HG23	0.69	1.61	5	4
1:A:93:ILE:HD11	1:A:95:ALA:HB2	0.69	1.64	24	2
1:A:63:LEU:N	1:A:72:ILE:HD13	0.69	2.01	7	17
1:B:85:ILE:N	1:B:85:ILE:HD13	0.69	2.01	15	6
1:A:32:VAL:HG12	1:A:84:ILE:HG13	0.69	1.63	16	3
1:A:15:ILE:HG22	1:A:62:ILE:CG2	0.69	2.17	24	1
1:A:63:LEU:HD12	1:A:71:ALA:O	0.69	1.88	7	2
1:B:87:ARG:O	1:B:91:THR:HG23	0.69	1.86	14	4
1:A:81:PRO:O	1:A:82:VAL:HG23	0.68	1.88	17	11
1:A:91:THR:HG21	1:B:6:TRP:CG	0.68	2.23	13	1
1:A:63:LEU:HD22	1:A:71:ALA:O	0.68	1.88	24	4
1:A:62:ILE:HG21	1:A:75:VAL:HG21	0.68	1.65	24	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ILE:HG22	1:A:66:ILE:CG1	0.68	2.17	5	6
1:B:76:LEU:N	1:B:76:LEU:HD22	0.68	2.03	22	1
1:A:84:ILE:C	1:A:85:ILE:HD13	0.68	2.09	27	8
1:A:4:THR:C	1:A:5:LEU:HD23	0.68	2.09	4	1
1:B:22:ALA:HB1	1:B:85:ILE:HD11	0.68	1.66	8	10
1:A:5:LEU:HD22	1:B:26:THR:CG2	0.68	2.18	11	1
1:A:36:MET:SD	1:A:38:LEU:HD13	0.68	2.28	5	2
1:A:42:TRP:CD1	1:A:59:TYR:CE1	0.68	2.81	28	10
1:B:63:LEU:HD22	1:B:71:ALA:O	0.68	1.88	17	5
1:B:34:GLU:HA	1:B:80:THR:HG22	0.68	1.64	10	14
1:A:86:GLY:O	1:A:90:LEU:HD22	0.68	1.89	7	1
1:A:5:LEU:HD12	1:B:87:ARG:HG3	0.68	1.64	27	1
1:A:63:LEU:HD11	1:A:70:LYS:CG	0.68	2.18	4	3
1:A:5:LEU:CD2	1:B:91:THR:HG23	0.68	2.19	21	1
1:A:4:THR:HG22	1:B:96:THR:HG22	0.68	1.65	1	7
1:A:11:VAL:HG23	1:A:13:ILE:CG2	0.68	2.19	14	6
1:A:26:THR:HG23	1:A:90:LEU:HD12	0.68	1.65	28	1
1:B:99:PHE:N	1:B:99:PHE:CD1	0.67	2.61	4	9
1:A:38:LEU:HD22	1:A:62:ILE:HD12	0.67	1.65	17	1
1:B:35:GLU:HA	1:B:77:VAL:HG12	0.67	1.64	14	8
1:A:4:THR:O	1:A:5:LEU:HD12	0.67	1.88	9	1
1:B:11:VAL:CG2	1:B:66:ILE:HG23	0.67	2.19	10	1
1:A:97:LEU:CD1	1:B:97:LEU:HD11	0.67	2.19	13	19
1:A:15:ILE:HD12	1:A:33:LEU:CD2	0.67	2.20	20	13
1:A:24:LEU:HD23	1:A:85:ILE:HB	0.67	1.64	26	5
1:A:97:LEU:HD21	1:B:26:THR:OG1	0.67	1.90	16	3
1:B:87:ARG:N	1:B:90:LEU:HD22	0.67	2.04	20	3
1:B:45:LYS:NZ	1:B:56:VAL:HG23	0.67	2.04	26	2
1:B:15:ILE:CG2	1:B:62:ILE:HG21	0.67	2.18	18	5
1:B:31:THR:HA	1:B:84:ILE:O	0.67	1.90	21	20
1:A:91:THR:HG21	1:B:6:TRP:CD2	0.67	2.25	13	1
1:A:14:LYS:HD2	1:A:19:LEU:HD21	0.67	1.67	6	2
1:A:99:PHE:CG	1:B:93:ILE:CD1	0.67	2.78	18	2
1:A:64:ILE:HG23	1:A:89:LEU:HD11	0.67	1.64	17	1
1:A:66:ILE:HD11	1:A:89:LEU:HD12	0.67	1.65	17	1
1:B:5:LEU:HD13	1:B:9:PRO:HA	0.67	1.67	10	1
1:A:88:ASN:HD21	1:A:89:LEU:HD23	0.66	1.49	22	11
1:B:48:GLY:CA	1:B:53:PHE:CD2	0.66	2.78	20	8
1:B:5:LEU:HD22	1:B:5:LEU:N	0.66	2.04	25	4
1:B:90:LEU:N	1:B:90:LEU:HD12	0.66	2.06	22	3
1:B:86:GLY:C	1:B:90:LEU:HD13	0.66	2.11	22	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:81:PRO:O	1:B:82:VAL:HG23	0.66	1.90	13	18
1:B:64:ILE:HG22	1:B:71:ALA:O	0.66	1.90	5	17
1:B:64:ILE:CD1	1:B:66:ILE:HD11	0.66	2.20	26	11
1:B:99:PHE:CD1	1:B:99:PHE:N	0.66	2.64	21	11
1:B:53:PHE:CD1	1:B:53:PHE:N	0.66	2.64	7	11
1:B:58:GLN:CD	1:B:74:THR:HG21	0.66	2.10	22	1
1:B:38:LEU:CD1	1:B:77:VAL:HG21	0.66	2.20	12	3
1:A:63:LEU:HD23	1:A:63:LEU:C	0.66	2.11	4	2
1:A:97:LEU:HD11	1:B:97:LEU:CD1	0.66	2.21	1	20
1:A:47:ILE:HD11	1:A:54:ILE:CD1	0.66	2.20	10	4
1:B:30:ASP:CB	1:B:76:LEU:HD11	0.66	2.21	17	4
1:B:42:TRP:CD1	1:B:59:TYR:CZ	0.66	2.84	14	10
1:B:5:LEU:O	1:B:7:GLN:N	0.66	2.29	15	19
1:B:89:LEU:HD22	1:B:92:GLN:OE1	0.66	1.91	26	3
1:B:64:ILE:HG23	1:B:89:LEU:HD11	0.66	1.68	9	3
1:B:13:ILE:CG2	1:B:22:ALA:HB2	0.66	2.21	27	6
1:B:63:LEU:HD13	1:B:63:LEU:C	0.66	2.12	27	9
1:A:59:TYR:C	1:A:62:ILE:HD11	0.65	2.12	11	4
1:A:24:LEU:HD22	1:A:90:LEU:HD21	0.65	1.67	4	2
1:B:38:LEU:HD23	1:B:59:TYR:CD2	0.65	2.27	7	3
1:A:63:LEU:HD11	1:A:70:LYS:HG3	0.65	1.69	4	2
1:A:10:LEU:HD22	1:A:21:GLU:HB3	0.65	1.69	19	10
1:A:99:PHE:CD1	1:A:99:PHE:N	0.65	2.64	4	7
1:B:45:LYS:O	1:B:56:VAL:HG23	0.65	1.91	25	2
1:A:47:ILE:HD12	1:B:50:ILE:HG21	0.65	1.67	14	17
1:A:5:LEU:O	1:B:91:THR:HG23	0.65	1.91	3	1
1:A:42:TRP:CD1	1:A:59:TYR:CZ	0.65	2.85	2	12
1:A:31:THR:HA	1:A:84:ILE:O	0.65	1.92	3	25
1:A:26:THR:HG23	1:A:90:LEU:CD1	0.65	2.22	17	3
1:A:48:GLY:CA	1:A:53:PHE:CD2	0.65	2.80	16	5
1:B:63:LEU:C	1:B:63:LEU:HD13	0.65	2.12	16	8
1:B:63:LEU:HD22	1:B:72:ILE:HG13	0.65	1.68	24	1
1:A:24:LEU:CD1	1:B:99:PHE:CZ	0.64	2.80	28	2
1:A:85:ILE:HG22	1:A:85:ILE:O	0.64	1.93	16	4
1:A:5:LEU:HD11	1:B:26:THR:HG23	0.64	1.68	10	1
1:A:5:LEU:HD23	1:B:87:ARG:HB3	0.64	1.68	18	1
1:B:13:ILE:HG21	1:B:22:ALA:HB2	0.64	1.70	27	2
1:A:99:PHE:N	1:A:99:PHE:CD1	0.64	2.64	19	14
1:A:63:LEU:C	1:A:63:LEU:HD12	0.64	2.13	23	2
1:A:53:PHE:N	1:A:53:PHE:CD1	0.64	2.64	6	9
1:B:88:ASN:C	1:B:89:LEU:HD23	0.64	2.13	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:TRP:CD1	1:A:59:TYR:CE2	0.64	2.85	19	1
1:B:33:LEU:HB2	1:B:75:VAL:HG12	0.64	1.68	21	4
1:B:15:ILE:HD13	1:B:75:VAL:CG1	0.64	2.22	19	6
1:B:24:LEU:HD23	1:B:85:ILE:HB	0.64	1.70	15	4
1:B:13:ILE:HG12	1:B:22:ALA:HB2	0.64	1.70	11	4
1:B:14:LYS:HG3	1:B:19:LEU:HD21	0.64	1.70	1	1
1:B:3:VAL:HG12	1:B:5:LEU:H	0.64	1.52	5	1
1:A:26:THR:HA	1:A:90:LEU:HD21	0.64	1.68	6	1
1:A:82:VAL:CG1	1:A:84:ILE:CG1	0.64	2.75	20	2
1:A:15:ILE:HG22	1:A:38:LEU:HD13	0.64	1.69	23	2
1:A:83:ASN:OD1	1:A:83:ASN:N	0.64	2.30	8	7
1:A:59:TYR:O	1:A:74:THR:HG23	0.64	1.92	8	2
1:A:39:PRO:O	1:A:59:TYR:CE1	0.64	2.50	22	5
1:A:50:ILE:CG2	1:B:47:ILE:HD12	0.64	2.22	2	2
1:A:68:GLY:O	1:A:69:HIS:CG	0.64	2.50	17	1
1:A:63:LEU:C	1:A:63:LEU:HD13	0.63	2.14	2	6
1:A:87:ARG:N	1:A:90:LEU:HD22	0.63	2.09	25	1
1:A:3:VAL:HG12	1:A:3:VAL:O	0.63	1.93	12	1
1:B:38:LEU:HD23	1:B:59:TYR:CG	0.63	2.29	22	4
1:B:76:LEU:HD12	1:B:76:LEU:N	0.63	2.08	15	2
1:B:13:ILE:HG22	1:B:66:ILE:CG1	0.63	2.23	9	6
1:A:25:ASP:CB	1:A:84:ILE:CG2	0.63	2.77	20	11
1:A:82:VAL:CG1	1:A:84:ILE:HD11	0.63	2.24	20	9
1:A:50:ILE:HG23	1:B:54:ILE:CD1	0.63	2.23	20	7
1:B:31:THR:HG23	1:B:84:ILE:O	0.63	1.93	12	6
1:B:4:THR:O	1:B:6:TRP:N	0.63	2.32	26	17
1:B:87:ARG:HA	1:B:90:LEU:HD13	0.63	1.71	17	1
1:A:13:ILE:HG23	1:A:22:ALA:CB	0.63	2.23	17	6
1:B:53:PHE:N	1:B:53:PHE:CD1	0.63	2.67	20	12
1:B:34:GLU:N	1:B:80:THR:HG22	0.63	2.08	17	8
1:A:54:ILE:HD13	1:B:50:ILE:HG23	0.63	1.70	3	2
1:B:71:ALA:HB1	1:B:92:GLN:HE21	0.63	1.54	26	3
1:A:85:ILE:N	1:A:85:ILE:CD1	0.63	2.62	8	14
1:A:53:PHE:CD1	1:A:53:PHE:N	0.63	2.67	8	15
1:A:68:GLY:O	1:A:69:HIS:CD2	0.63	2.52	17	2
1:A:71:ALA:HB1	1:A:92:GLN:NE2	0.63	2.08	17	1
1:A:11:VAL:CB	1:A:66:ILE:HG23	0.62	2.24	6	1
1:A:45:LYS:CE	1:A:76:LEU:CD2	0.62	2.76	20	1
1:A:47:ILE:HG12	1:A:54:ILE:HD11	0.62	1.69	11	1
1:B:58:GLN:NE2	1:B:74:THR:HG21	0.62	2.09	22	1
1:B:38:LEU:HD12	1:B:39:PRO:HD3	0.62	1.69	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:N	1:A:62:ILE:HD12	0.62	2.09	2	2
1:B:86:GLY:O	1:B:90:LEU:HD22	0.62	1.94	19	1
1:A:45:LYS:HB2	1:A:56:VAL:HG23	0.62	1.72	12	1
1:A:93:ILE:CD1	1:B:99:PHE:CG	0.62	2.81	19	8
1:B:26:THR:HG23	1:B:90:LEU:HD22	0.62	1.72	17	1
1:A:13:ILE:HG23	1:A:22:ALA:HB2	0.62	1.72	27	4
1:B:89:LEU:HD13	1:B:92:GLN:NE2	0.62	2.10	22	3
1:A:31:THR:HG23	1:A:85:ILE:HD12	0.62	1.70	5	6
1:A:85:ILE:HG22	1:A:90:LEU:CD1	0.62	2.25	25	2
1:A:38:LEU:CB	1:A:59:TYR:CE1	0.62	2.82	18	3
1:A:54:ILE:CD1	1:B:50:ILE:HG23	0.62	2.25	25	3
1:A:83:ASN:N	1:A:83:ASN:OD1	0.62	2.32	2	8
1:B:15:ILE:HD12	1:B:33:LEU:HD22	0.62	1.70	27	4
1:B:13:ILE:HG21	1:B:22:ALA:CB	0.62	2.25	4	2
1:B:38:LEU:HB3	1:B:39:PRO:HD2	0.61	1.71	12	9
1:A:5:LEU:O	1:A:7:GLN:N	0.61	2.32	16	21
1:A:13:ILE:HG12	1:A:22:ALA:HB2	0.61	1.72	21	2
1:A:63:LEU:CD2	1:A:70:LYS:CG	0.61	2.78	15	1
1:B:25:ASP:OD2	1:B:28:ALA:HB2	0.61	1.94	19	3
1:B:14:LYS:HG3	1:B:19:LEU:HD12	0.61	1.72	12	1
1:B:76:LEU:N	1:B:76:LEU:CD2	0.61	2.63	22	1
1:A:82:VAL:HG12	1:A:84:ILE:HD11	0.61	1.72	23	8
1:A:63:LEU:HD22	1:A:72:ILE:HG12	0.61	1.72	10	1
1:A:99:PHE:CD2	1:B:93:ILE:CD1	0.61	2.84	21	15
1:A:76:LEU:N	1:A:76:LEU:HD12	0.61	2.09	20	2
1:B:13:ILE:HD12	1:B:15:ILE:HG13	0.61	1.72	15	5
1:B:82:VAL:HG13	1:B:83:ASN:N	0.61	2.11	1	8
1:B:24:LEU:CD2	1:B:90:LEU:HD21	0.61	2.26	28	1
1:B:38:LEU:HD12	1:B:39:PRO:HD2	0.61	1.73	18	6
1:A:97:LEU:CD1	1:B:97:LEU:CD1	0.61	2.78	3	21
1:A:15:ILE:HD13	1:A:75:VAL:HG21	0.61	1.71	6	5
1:A:13:ILE:CG2	1:A:22:ALA:HB2	0.61	2.25	1	9
1:B:80:THR:HG23	1:B:82:VAL:O	0.61	1.96	24	9
1:B:83:ASN:N	1:B:83:ASN:OD1	0.61	2.34	20	7
1:B:13:ILE:HG23	1:B:22:ALA:CB	0.61	2.26	13	4
1:A:34:GLU:N	1:A:80:THR:CG2	0.61	2.64	21	13
1:B:25:ASP:CB	1:B:84:ILE:CG2	0.61	2.79	14	16
1:A:4:THR:O	1:A:5:LEU:CB	0.61	2.48	9	6
1:A:82:VAL:HG12	1:A:84:ILE:CG1	0.61	2.25	14	2
1:A:48:GLY:CA	1:A:53:PHE:CD1	0.61	2.84	6	1
1:A:89:LEU:CD1	1:A:92:GLN:OE1	0.61	2.42	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:HIS:CB	1:A:93:ILE:HG22	0.61	2.26	2	2
1:A:99:PHE:CE1	1:B:1:PRO:O	0.60	2.54	28	13
1:A:96:THR:HG22	1:B:4:THR:HG23	0.60	1.71	13	6
1:A:68:GLY:O	1:A:69:HIS:CB	0.60	2.49	17	1
1:B:32:VAL:HG23	1:B:76:LEU:HB2	0.60	1.73	18	8
1:A:28:ALA:HB2	2:B:100:DMP:C25	0.60	2.26	11	8
1:B:13:ILE:HD12	1:B:15:ILE:HD12	0.60	1.73	20	2
1:A:91:THR:HG22	1:B:6:TRP:HB3	0.60	1.72	17	1
1:B:3:VAL:HG13	1:B:5:LEU:HD23	0.60	1.73	3	1
1:B:32:VAL:HG12	1:B:84:ILE:HG12	0.60	1.72	6	7
1:A:15:ILE:HG22	1:A:38:LEU:HD21	0.60	1.72	28	4
1:A:54:ILE:HD12	1:A:56:VAL:HG13	0.60	1.71	23	1
1:A:85:ILE:CD1	1:A:85:ILE:N	0.60	2.65	21	10
1:B:85:ILE:CD1	1:B:85:ILE:N	0.60	2.63	1	6
1:A:85:ILE:HG23	1:A:89:LEU:CB	0.60	2.27	5	3
1:A:6:TRP:CE3	1:B:91:THR:HG21	0.60	2.31	6	3
1:B:5:LEU:HD22	1:B:5:LEU:H	0.60	1.57	9	1
1:B:59:TYR:C	1:B:62:ILE:HD11	0.60	2.15	4	3
1:B:11:VAL:HG21	1:B:66:ILE:CG2	0.60	2.25	10	1
1:B:4:THR:O	1:B:5:LEU:C	0.60	2.39	10	16
1:B:61:GLN:HA	1:B:72:ILE:HG23	0.60	1.73	23	9
1:B:90:LEU:N	1:B:90:LEU:HD23	0.60	2.11	10	1
1:B:31:THR:CG2	1:B:33:LEU:CD1	0.60	2.80	13	7
1:B:63:LEU:CD1	1:B:63:LEU:C	0.60	2.69	24	6
1:A:41:ARG:O	1:A:59:TYR:CD1	0.60	2.54	5	2
1:B:5:LEU:HD22	1:B:6:TRP:N	0.60	2.11	1	2
1:A:4:THR:O	1:A:5:LEU:HB3	0.60	1.95	9	1
1:A:63:LEU:HD12	1:A:71:ALA:C	0.60	2.16	15	1
1:A:50:ILE:CD1	2:B:100:DMP:C76	0.60	2.79	22	27
1:B:63:LEU:N	1:B:72:ILE:CD1	0.60	2.65	22	8
1:B:10:LEU:HD23	1:B:22:ALA:N	0.60	2.12	4	3
1:B:64:ILE:CG2	1:B:89:LEU:CD1	0.60	2.80	10	7
1:B:26:THR:HA	1:B:90:LEU:HD21	0.60	1.72	14	2
1:B:85:ILE:N	1:B:85:ILE:CD1	0.60	2.64	5	8
1:A:5:LEU:CD2	1:B:26:THR:HG21	0.60	2.27	11	1
1:A:5:LEU:HD21	1:B:97:LEU:HD13	0.60	1.72	11	2
1:B:12:THR:CG2	1:B:19:LEU:HD23	0.59	2.27	12	2
1:A:13:ILE:HG21	1:A:22:ALA:CB	0.59	2.27	19	6
1:B:13:ILE:HG23	1:B:22:ALA:HB2	0.59	1.73	13	3
1:B:39:PRO:O	1:B:59:TYR:CE1	0.59	2.55	24	4
1:A:90:LEU:HD23	1:A:93:ILE:HD11	0.59	1.72	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:VAL:HG21	1:A:76:LEU:HD23	0.59	1.74	28	2
1:B:83:ASN:OD1	1:B:83:ASN:N	0.59	2.34	4	9
1:A:76:LEU:H	1:A:76:LEU:HD12	0.59	1.57	7	3
1:A:11:VAL:HB	1:A:66:ILE:HG23	0.59	1.74	6	1
1:A:5:LEU:HD23	1:B:91:THR:CG2	0.59	2.27	21	1
1:A:38:LEU:HB2	1:A:59:TYR:CE1	0.59	2.32	18	2
1:B:84:ILE:HD11	2:B:100:DMP:C31	0.59	2.27	17	3
1:A:83:ASN:O	1:A:84:ILE:CG1	0.59	2.50	20	2
1:A:98:ASN:ND2	1:B:2:GLN:CG	0.59	2.66	16	18
1:B:88:ASN:ND2	1:B:89:LEU:CD2	0.59	2.64	23	18
1:A:42:TRP:CD1	1:A:59:TYR:OH	0.59	2.55	16	7
1:A:50:ILE:CG2	1:B:47:ILE:HD11	0.59	2.28	15	5
1:A:32:VAL:HG12	1:A:84:ILE:HG12	0.59	1.73	1	10
1:A:1:PRO:O	1:B:99:PHE:CE1	0.59	2.55	10	7
1:B:9:PRO:O	1:B:24:LEU:HD12	0.59	1.97	23	1
1:B:4:THR:O	1:B:5:LEU:HD23	0.59	1.96	20	1
1:A:5:LEU:HD11	1:B:97:LEU:CD1	0.59	2.27	3	1
1:B:60:ASP:O	1:B:61:GLN:CB	0.59	2.50	25	22
1:A:54:ILE:CG2	1:B:51:GLY:N	0.59	2.65	18	12
1:B:31:THR:N	1:B:88:ASN:OD1	0.59	2.35	9	11
1:B:42:TRP:CD1	1:B:59:TYR:OH	0.59	2.56	14	7
1:A:38:LEU:HD12	1:A:77:VAL:CG2	0.59	2.25	25	6
1:B:36:MET:SD	1:B:38:LEU:HD13	0.59	2.37	22	2
1:A:15:ILE:CG2	1:A:62:ILE:CG2	0.59	2.80	24	1
1:B:24:LEU:CD2	1:B:85:ILE:CG2	0.59	2.81	27	1
1:B:85:ILE:HG22	1:B:85:ILE:O	0.59	1.98	6	4
1:B:58:GLN:CG	1:B:74:THR:CG2	0.59	2.81	16	6
1:B:8:ARG:CD	1:B:23:LEU:HD13	0.59	2.24	5	1
1:A:66:ILE:CD1	1:A:89:LEU:HD12	0.59	2.28	17	1
1:B:13:ILE:HD13	1:B:15:ILE:HD11	0.59	1.74	15	1
1:B:14:LYS:HE2	1:B:19:LEU:HD11	0.59	1.75	5	2
1:B:67:CYS:O	1:B:69:HIS:CD2	0.59	2.56	17	5
1:A:12:THR:CG2	1:A:19:LEU:HD23	0.59	2.27	23	3
1:B:97:LEU:O	1:B:99:PHE:CE1	0.59	2.56	3	6
1:A:99:PHE:CD1	1:B:95:ALA:CB	0.59	2.85	8	1
1:B:13:ILE:CG2	1:B:22:ALA:CB	0.59	2.81	4	7
1:A:64:ILE:CG2	1:A:89:LEU:CD1	0.59	2.81	21	3
1:A:31:THR:HG22	1:A:31:THR:O	0.59	1.97	17	5
1:B:38:LEU:CB	1:B:39:PRO:CD	0.59	2.80	6	4
1:B:15:ILE:CG2	1:B:36:MET:CE	0.59	2.81	2	3
1:B:48:GLY:HA3	1:B:53:PHE:CD2	0.59	2.33	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ILE:HD12	1:A:54:ILE:O	0.59	1.98	11	1
1:A:96:THR:CG2	1:B:4:THR:HG22	0.59	2.28	17	1
1:B:38:LEU:HB2	1:B:59:TYR:CE2	0.59	2.33	18	2
1:B:50:ILE:CD1	2:B:100:DMP:C26	0.58	2.80	14	28
1:B:38:LEU:O	1:B:59:TYR:CZ	0.58	2.56	16	1
1:A:38:LEU:HD12	1:A:59:TYR:CD2	0.58	2.33	28	2
1:B:30:ASP:CB	1:B:76:LEU:CD1	0.58	2.81	8	2
1:A:2:GLN:CG	1:B:98:ASN:ND2	0.58	2.65	22	19
1:B:86:GLY:C	1:B:90:LEU:HD22	0.58	2.18	21	3
1:B:87:ARG:N	1:B:90:LEU:CD1	0.58	2.66	17	1
1:A:45:LYS:NZ	1:A:56:VAL:HG23	0.58	2.13	20	1
1:B:76:LEU:H	1:B:76:LEU:HD12	0.58	1.59	3	3
1:A:48:GLY:HA3	1:A:53:PHE:CD2	0.58	2.33	16	14
1:B:82:VAL:HG13	1:B:83:ASN:O	0.58	1.97	21	3
1:A:91:THR:CG2	1:B:5:LEU:HD23	0.58	2.28	1	1
1:B:38:LEU:CB	1:B:59:TYR:CE2	0.58	2.86	18	3
1:B:5:LEU:H	1:B:5:LEU:HD13	0.58	1.57	26	1
1:A:34:GLU:CG	1:A:80:THR:O	0.58	2.52	8	4
1:B:48:GLY:HA2	1:B:53:PHE:CD1	0.58	2.34	8	2
1:B:66:ILE:O	1:B:69:HIS:CD2	0.58	2.57	25	1
1:B:63:LEU:CD1	1:B:71:ALA:N	0.58	2.66	3	1
1:A:88:ASN:ND2	1:A:89:LEU:CD2	0.58	2.63	1	22
1:B:12:THR:CG2	1:B:19:LEU:CD2	0.58	2.81	26	2
1:A:22:ALA:HB1	1:A:85:ILE:HD11	0.58	1.76	26	4
1:A:14:LYS:HE2	1:A:19:LEU:HD11	0.58	1.75	23	1
1:A:56:VAL:HG12	1:A:78:GLY:CA	0.58	2.27	20	4
1:B:85:ILE:HD13	1:B:85:ILE:N	0.58	2.12	8	7
1:B:38:LEU:HB3	1:B:59:TYR:CE1	0.58	2.34	4	4
1:B:64:ILE:HG21	1:B:89:LEU:HD11	0.58	1.74	13	4
1:B:15:ILE:CD1	1:B:33:LEU:HD22	0.58	2.28	27	3
1:A:30:ASP:CB	1:A:88:ASN:OD1	0.58	2.52	5	2
1:A:67:CYS:O	1:A:69:HIS:CD2	0.58	2.56	3	6
1:A:90:LEU:N	1:A:90:LEU:CD1	0.58	2.67	25	1
1:B:34:GLU:CA	1:B:80:THR:HG22	0.58	2.28	10	5
1:A:23:LEU:O	1:A:25:ASP:N	0.58	2.37	17	18
1:A:47:ILE:HD11	1:B:50:ILE:CG2	0.58	2.28	2	6
1:A:12:THR:HG22	1:A:19:LEU:CD2	0.58	2.24	26	4
1:A:51:GLY:N	1:B:54:ILE:CG2	0.58	2.67	4	13
1:B:55:LYS:O	1:B:79:PRO:CD	0.58	2.51	26	27
1:A:4:THR:O	1:A:6:TRP:N	0.58	2.37	5	12
1:A:20:LYS:HB3	1:A:83:ASN:ND2	0.58	2.14	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:PHE:CD1	1:B:1:PRO:O	0.58	2.57	11	8
1:B:87:ARG:NH2	1:B:87:ARG:N	0.58	2.52	16	1
1:B:45:LYS:CE	1:B:56:VAL:CG2	0.58	2.80	26	1
1:A:48:GLY:HA2	1:A:53:PHE:CD1	0.57	2.34	6	3
1:B:84:ILE:CD1	2:B:100:DMP:C32	0.57	2.80	17	3
1:A:7:GLN:O	1:B:87:ARG:CD	0.57	2.53	3	1
1:A:63:LEU:C	1:A:63:LEU:HD23	0.57	2.19	27	1
1:B:21:GLU:O	1:B:83:ASN:CB	0.57	2.53	14	6
1:A:15:ILE:HG22	1:A:62:ILE:HG22	0.57	1.75	24	1
1:A:13:ILE:CG2	1:A:22:ALA:CB	0.57	2.83	1	9
1:A:64:ILE:CG2	1:A:71:ALA:O	0.57	2.53	8	14
1:A:54:ILE:HD13	1:A:56:VAL:HG13	0.57	1.74	11	1
1:B:26:THR:HG22	1:B:87:ARG:NH2	0.57	2.14	5	1
1:B:13:ILE:CD1	1:B:15:ILE:HD11	0.57	2.28	15	1
1:A:50:ILE:HG23	1:B:54:ILE:HG12	0.57	1.75	4	1
1:A:22:ALA:CB	1:A:85:ILE:CD1	0.57	2.80	12	2
1:A:30:ASP:O	1:A:86:GLY:HA3	0.57	2.00	5	21
1:B:82:VAL:CG1	1:B:83:ASN:N	0.57	2.68	17	17
1:A:38:LEU:CD1	1:A:59:TYR:CD2	0.57	2.87	16	2
1:B:64:ILE:CG2	1:B:71:ALA:O	0.57	2.52	1	16
1:B:90:LEU:HA	1:B:93:ILE:HD11	0.57	1.76	16	1
1:B:86:GLY:O	1:B:88:ASN:N	0.57	2.38	7	5
1:B:30:ASP:HB3	1:B:76:LEU:CD1	0.57	2.29	4	7
1:B:42:TRP:HB3	1:B:59:TYR:CE1	0.57	2.34	22	17
1:A:38:LEU:CB	1:A:39:PRO:CD	0.57	2.83	19	5
1:A:45:LYS:HE2	1:A:76:LEU:HD23	0.57	1.75	15	2
1:B:64:ILE:HG21	1:B:89:LEU:CD1	0.57	2.28	16	4
1:B:5:LEU:N	1:B:5:LEU:CD2	0.57	2.67	9	2
1:A:42:TRP:CZ3	1:A:57:ARG:CD	0.57	2.88	18	3
1:A:45:LYS:NZ	1:A:56:VAL:CG2	0.57	2.68	20	1
1:B:63:LEU:HD11	1:B:71:ALA:N	0.57	2.14	3	1
1:B:82:VAL:HG12	1:B:84:ILE:CD1	0.57	2.28	28	7
1:A:97:LEU:HD21	1:B:26:THR:HG1	0.57	1.60	16	1
1:B:45:LYS:HB3	1:B:56:VAL:HG23	0.57	1.77	3	2
1:A:71:ALA:HB1	1:A:92:GLN:CD	0.57	2.20	17	1
1:B:25:ASP:HB3	1:B:84:ILE:CG2	0.57	2.30	24	16
1:A:38:LEU:HD12	1:A:39:PRO:HD2	0.57	1.76	20	4
1:A:4:THR:HG23	1:B:96:THR:HG22	0.57	1.75	19	3
1:B:38:LEU:HD13	1:B:59:TYR:CD1	0.57	2.35	19	1
1:B:90:LEU:CD1	1:B:90:LEU:N	0.57	2.68	14	3
1:A:1:PRO:O	1:B:99:PHE:CD1	0.57	2.57	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:CG1	1:A:54:ILE:CG1	0.57	2.81	28	9
1:B:5:LEU:O	1:B:6:TRP:C	0.57	2.43	26	20
1:A:38:LEU:HB3	1:A:59:TYR:CE1	0.57	2.35	1	7
1:B:5:LEU:HD13	1:B:5:LEU:N	0.57	2.14	1	2
1:A:93:ILE:CD1	1:B:99:PHE:CB	0.57	2.83	24	1
1:B:26:THR:HG23	1:B:90:LEU:CD1	0.57	2.30	9	3
1:B:32:VAL:O	1:B:32:VAL:HG12	0.57	2.00	3	1
1:A:93:ILE:CD1	1:B:99:PHE:CD2	0.56	2.87	23	7
1:A:4:THR:HG22	1:B:96:THR:CG2	0.56	2.30	12	1
1:A:48:GLY:HA3	1:A:53:PHE:CE2	0.56	2.35	13	13
1:B:63:LEU:CD2	1:B:70:LYS:CG	0.56	2.80	26	3
1:B:82:VAL:HG12	1:B:84:ILE:HD12	0.56	1.76	17	1
1:A:40:GLY:O	1:A:41:ARG:CB	0.56	2.53	12	8
1:B:40:GLY:O	1:B:41:ARG:CB	0.56	2.53	4	2
1:B:82:VAL:HG12	1:B:84:ILE:HD11	0.56	1.76	1	3
1:A:87:ARG:CB	1:A:87:ARG:CZ	0.56	2.82	5	1
1:B:87:ARG:HA	1:B:90:LEU:CD1	0.56	2.30	17	1
1:A:50:ILE:HD11	1:B:84:ILE:HD12	0.56	1.77	15	1
1:A:31:THR:CG2	1:A:33:LEU:CD1	0.56	2.83	12	7
1:A:55:LYS:O	1:A:79:PRO:CD	0.56	2.53	25	26
1:A:63:LEU:O	1:A:63:LEU:CD1	0.56	2.54	11	7
1:B:26:THR:HG23	1:B:90:LEU:CD2	0.56	2.27	14	1
1:B:38:LEU:HD13	1:B:59:TYR:CG	0.56	2.35	14	2
1:B:98:ASN:C	1:B:99:PHE:CD1	0.56	2.79	24	1
1:A:13:ILE:HD12	1:A:15:ILE:HD12	0.56	1.77	4	2
1:A:5:LEU:HD23	1:B:91:THR:CA	0.56	2.29	21	1
1:B:15:ILE:HD13	1:B:75:VAL:CG2	0.56	2.30	18	1
1:B:54:ILE:HD11	1:B:56:VAL:HG13	0.56	1.78	4	1
1:B:72:ILE:O	1:B:92:GLN:NE2	0.56	2.38	22	5
1:A:15:ILE:HD13	1:A:75:VAL:CG1	0.56	2.31	19	7
1:A:86:GLY:C	1:A:90:LEU:CD2	0.56	2.74	7	1
1:A:5:LEU:O	1:A:6:TRP:C	0.56	2.44	2	20
1:A:42:TRP:HB3	1:A:59:TYR:CZ	0.56	2.36	20	5
1:B:86:GLY:C	1:B:90:LEU:CD2	0.56	2.74	19	1
1:A:99:PHE:HZ	1:B:3:VAL:HG21	0.56	1.59	9	1
1:B:15:ILE:CG2	1:B:36:MET:HE2	0.56	2.30	2	1
1:A:63:LEU:C	1:A:63:LEU:HD22	0.56	2.21	3	3
1:A:5:LEU:CD2	1:B:91:THR:N	0.56	2.68	21	1
1:B:28:ALA:HB2	2:B:100:DMP:C75	0.56	2.29	4	7
1:B:80:THR:HG23	1:B:82:VAL:H	0.56	1.60	23	4
1:B:56:VAL:HG12	1:B:78:GLY:CA	0.56	2.31	26	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:VAL:HG13	1:A:83:ASN:N	0.56	2.16	22	7
1:B:38:LEU:HG	1:B:39:PRO:HD2	0.56	1.77	6	3
1:B:33:LEU:HD23	1:B:83:ASN:OD1	0.56	2.01	7	2
1:B:24:LEU:HD22	1:B:85:ILE:HG21	0.56	1.76	13	1
1:A:62:ILE:HD13	1:A:75:VAL:HG23	0.56	1.76	1	1
1:B:23:LEU:O	1:B:25:ASP:N	0.56	2.39	13	15
1:A:21:GLU:O	1:A:83:ASN:ND2	0.56	2.38	5	15
1:A:63:LEU:CD1	1:A:71:ALA:O	0.56	2.54	7	2
1:A:38:LEU:HB3	1:A:59:TYR:CZ	0.56	2.36	15	5
1:A:5:LEU:CD2	1:B:26:THR:CG2	0.56	2.83	11	1
1:A:59:TYR:CB	1:A:62:ILE:HD11	0.56	2.29	1	1
1:B:32:VAL:CG1	1:B:84:ILE:HD12	0.56	2.31	22	1
1:B:64:ILE:HG23	1:B:64:ILE:O	0.56	2.01	25	3
1:A:24:LEU:CD2	1:A:90:LEU:CD2	0.56	2.83	4	1
1:A:42:TRP:HB3	1:A:59:TYR:CD1	0.56	2.36	28	16
1:B:71:ALA:HB1	1:B:92:GLN:NE2	0.56	2.16	23	3
1:A:15:ILE:CG2	1:A:62:ILE:HG21	0.56	2.31	18	4
1:A:26:THR:O	1:A:87:ARG:NH2	0.56	2.39	17	1
1:B:26:THR:O	1:B:87:ARG:NH1	0.56	2.39	16	4
1:B:35:GLU:N	1:B:78:GLY:O	0.56	2.39	3	15
1:B:21:GLU:O	1:B:83:ASN:ND2	0.56	2.38	27	10
1:A:33:LEU:CD2	1:A:83:ASN:OD1	0.56	2.53	1	1
1:A:22:ALA:HB1	1:A:85:ILE:HG12	0.56	1.78	28	2
1:A:64:ILE:HD11	1:A:66:ILE:HD11	0.56	1.78	2	1
1:A:5:LEU:HD11	1:B:87:ARG:HG2	0.56	1.77	21	1
1:B:20:LYS:HB3	1:B:83:ASN:ND2	0.56	2.15	19	6
1:B:3:VAL:HG11	1:B:9:PRO:HB3	0.56	1.77	1	4
1:A:25:ASP:OD2	1:A:28:ALA:HB2	0.56	2.01	5	2
1:B:85:ILE:HG22	1:B:90:LEU:CD2	0.56	2.31	10	1
1:A:82:VAL:CG1	1:A:84:ILE:HG13	0.55	2.31	20	4
1:B:30:ASP:O	1:B:86:GLY:HA3	0.55	2.00	8	24
1:B:33:LEU:HD13	1:B:75:VAL:HG11	0.55	1.75	24	1
1:B:71:ALA:HB1	1:B:89:LEU:CD1	0.55	2.31	15	3
1:B:45:LYS:HZ1	1:B:76:LEU:HD23	0.55	1.58	26	2
1:B:87:ARG:CZ	1:B:90:LEU:HB2	0.55	2.31	27	1
1:A:97:LEU:O	1:A:99:PHE:CE1	0.55	2.59	17	6
1:A:5:LEU:HD11	1:A:9:PRO:HD3	0.55	1.78	27	1
1:A:5:LEU:HB3	1:B:87:ARG:CZ	0.55	2.31	27	1
1:A:25:ASP:HB3	1:A:84:ILE:CG2	0.55	2.32	20	15
1:A:12:THR:HG21	1:A:19:LEU:HD23	0.55	1.77	11	2
1:A:86:GLY:C	1:A:90:LEU:HD13	0.55	2.22	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:TRP:N	1:A:42:TRP:CD1	0.55	2.74	17	4
1:A:63:LEU:CD2	1:A:71:ALA:O	0.55	2.54	24	2
1:B:87:ARG:CA	1:B:90:LEU:HD13	0.55	2.32	17	2
1:B:11:VAL:HG21	1:B:66:ILE:CG1	0.55	2.31	27	3
1:B:85:ILE:CG2	1:B:89:LEU:CB	0.55	2.85	23	4
1:B:63:LEU:O	1:B:63:LEU:CD1	0.55	2.55	16	10
1:B:38:LEU:HB3	1:B:59:TYR:CZ	0.55	2.36	8	2
1:B:45:LYS:O	1:B:56:VAL:CG2	0.55	2.54	27	6
1:A:37:SER:C	1:A:38:LEU:HD22	0.55	2.21	1	1
1:A:15:ILE:CG2	1:A:62:ILE:HG22	0.55	2.31	24	1
1:B:11:VAL:HG11	1:B:24:LEU:HD21	0.55	1.78	10	1
1:A:87:ARG:O	1:A:91:THR:CG2	0.55	2.55	17	1
1:A:26:THR:O	1:A:87:ARG:NH1	0.55	2.39	3	1
1:A:45:LYS:CB	1:A:56:VAL:CG2	0.55	2.83	12	1
1:B:84:ILE:HD11	2:B:100:DMP:H32	0.55	1.78	22	1
1:B:38:LEU:HB3	1:B:59:TYR:CD2	0.55	2.36	26	1
1:A:63:LEU:HD13	1:A:72:ILE:HG13	0.55	1.79	15	1
1:A:60:ASP:O	1:A:61:GLN:CB	0.55	2.55	19	22
1:B:61:GLN:HA	1:B:72:ILE:CG2	0.55	2.31	3	19
1:B:38:LEU:CB	1:B:59:TYR:CD2	0.55	2.90	26	1
1:A:50:ILE:CG1	2:B:100:DMP:H32	0.55	2.32	2	23
1:A:63:LEU:CD1	1:A:63:LEU:O	0.55	2.54	28	7
1:B:15:ILE:HG23	1:B:62:ILE:HG22	0.55	1.79	14	2
1:A:42:TRP:CG	1:A:59:TYR:CZ	0.55	2.95	19	1
1:B:38:LEU:CD1	1:B:39:PRO:CD	0.55	2.84	18	5
1:B:64:ILE:O	1:B:71:ALA:HB3	0.55	2.02	28	2
1:B:32:VAL:HG12	1:B:84:ILE:HG13	0.55	1.76	26	1
1:A:40:GLY:O	1:A:41:ARG:HB2	0.55	2.02	28	9
1:B:48:GLY:CA	1:B:53:PHE:CD1	0.55	2.90	8	2
1:A:13:ILE:HG21	1:A:22:ALA:HB2	0.55	1.78	19	3
1:A:69:HIS:CD2	1:A:69:HIS:N	0.55	2.73	1	1
1:A:38:LEU:HG	1:A:39:PRO:HD2	0.55	1.77	6	6
1:B:31:THR:HG22	1:B:31:THR:O	0.55	2.00	19	2
1:A:42:TRP:CD1	1:A:42:TRP:N	0.55	2.75	19	1
1:A:30:ASP:CB	1:A:76:LEU:HD11	0.55	2.32	17	2
1:A:95:ALA:O	1:B:5:LEU:HD11	0.55	2.02	5	1
1:B:45:LYS:HE2	1:B:56:VAL:HG23	0.55	1.74	26	2
1:B:13:ILE:CD1	1:B:15:ILE:CG1	0.55	2.83	15	1
1:B:58:GLN:HG3	1:B:74:THR:HG22	0.55	1.77	12	3
1:A:34:GLU:HA	1:A:80:THR:CG2	0.55	2.32	16	11
1:A:15:ILE:HG22	1:A:36:MET:CE	0.55	2.31	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ILE:O	1:A:68:GLY:N	0.55	2.40	21	3
1:B:5:LEU:CD2	1:B:6:TRP:N	0.55	2.70	1	2
1:A:42:TRP:CZ3	1:A:57:ARG:HD3	0.55	2.36	18	5
1:A:11:VAL:O	1:A:22:ALA:HB3	0.55	2.02	17	1
1:A:32:VAL:O	1:A:32:VAL:HG12	0.55	2.01	3	1
1:A:5:LEU:HD11	1:B:97:LEU:HD13	0.55	1.78	3	1
1:A:57:ARG:O	1:A:59:TYR:N	0.55	2.40	27	3
1:A:82:VAL:CG1	1:A:83:ASN:N	0.55	2.70	17	15
1:A:32:VAL:O	1:A:32:VAL:CG1	0.55	2.55	14	2
1:A:46:MET:CB	1:A:54:ILE:O	0.55	2.55	23	3
1:B:63:LEU:CD1	1:B:63:LEU:O	0.55	2.54	17	6
1:A:63:LEU:CD1	1:A:71:ALA:N	0.55	2.70	7	2
1:A:3:VAL:HG12	1:A:5:LEU:H	0.55	1.60	6	2
1:A:58:GLN:CG	1:A:60:ASP:OD1	0.55	2.55	10	1
1:A:5:LEU:HD12	1:B:87:ARG:CG	0.55	2.32	27	1
1:A:34:GLU:HA	1:A:80:THR:HG23	0.54	1.79	3	4
1:A:4:THR:O	1:A:5:LEU:C	0.54	2.46	24	12
1:B:81:PRO:O	1:B:82:VAL:CG2	0.54	2.55	22	2
1:A:34:GLU:CA	1:A:80:THR:HG22	0.54	2.32	12	4
1:B:36:MET:SD	1:B:37:SER:N	0.54	2.80	18	7
1:A:63:LEU:C	1:A:63:LEU:CD1	0.54	2.75	10	3
1:A:27:GLY:O	1:B:23:LEU:HD11	0.54	2.03	22	2
1:B:34:GLU:HA	1:B:80:THR:CG2	0.54	2.32	26	8
1:A:26:THR:O	1:A:87:ARG:CZ	0.54	2.56	17	1
1:B:87:ARG:CZ	1:B:90:LEU:CB	0.54	2.85	27	1
1:B:28:ALA:CB	2:B:100:DMP:C75	0.54	2.86	4	9
1:B:98:ASN:N	1:B:98:ASN:ND2	0.54	2.54	1	7
1:B:31:THR:O	1:B:31:THR:HG22	0.54	2.01	23	5
1:A:15:ILE:HG22	1:A:36:MET:HE2	0.54	1.78	22	3
1:A:21:GLU:O	1:A:83:ASN:CB	0.54	2.56	13	7
1:A:31:THR:OG1	1:A:88:ASN:ND2	0.54	2.41	22	2
1:B:64:ILE:HD13	1:B:66:ILE:CD1	0.54	2.32	2	2
1:A:5:LEU:HD23	1:B:91:THR:HA	0.54	1.79	21	1
1:A:24:LEU:HD22	1:A:90:LEU:CD2	0.54	2.31	4	1
1:A:28:ALA:CB	2:B:100:DMP:C25	0.54	2.85	10	9
1:B:35:GLU:HA	1:B:77:VAL:CG1	0.54	2.33	6	7
1:B:58:GLN:HG3	1:B:74:THR:CG2	0.54	2.31	5	8
1:B:11:VAL:HG12	1:B:67:CYS:SG	0.54	2.42	17	1
1:B:5:LEU:HD23	1:B:9:PRO:HA	0.54	1.80	21	1
1:A:15:ILE:CD1	1:A:75:VAL:CG2	0.54	2.82	22	2
1:A:93:ILE:CD1	1:A:95:ALA:HB2	0.54	2.32	24	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:56:VAL:HG12	1:B:78:GLY:N	0.54	2.18	15	3
1:A:60:ASP:CG	1:A:74:THR:HG23	0.54	2.21	15	1
1:A:38:LEU:O	1:A:59:TYR:CZ	0.54	2.61	21	1
1:A:38:LEU:HD13	1:A:59:TYR:CD2	0.54	2.37	24	2
1:A:6:TRP:CD2	1:B:91:THR:HB	0.54	2.38	13	1
1:B:62:ILE:CD1	1:B:75:VAL:HG23	0.54	2.28	17	1
1:B:36:MET:HE2	1:B:38:LEU:HD21	0.54	1.78	15	1
1:A:63:LEU:CD2	1:A:63:LEU:C	0.54	2.76	4	3
1:B:40:GLY:O	1:B:41:ARG:CG	0.54	2.56	18	2
1:B:55:LYS:O	1:B:79:PRO:HD2	0.54	2.03	25	23
1:B:36:MET:SD	1:B:38:LEU:CD1	0.54	2.96	22	1
1:B:87:ARG:N	1:B:90:LEU:HD13	0.54	2.18	22	2
1:B:32:VAL:HA	1:B:76:LEU:HB2	0.54	1.80	22	6
1:B:47:ILE:HD11	1:B:54:ILE:CD1	0.54	2.33	7	8
1:A:32:VAL:CG1	1:A:84:ILE:CG1	0.54	2.86	6	7
1:B:42:TRP:CE3	1:B:57:ARG:HG2	0.54	2.38	11	1
1:A:34:GLU:CB	1:A:80:THR:O	0.54	2.56	20	1
1:B:85:ILE:CG2	1:B:90:LEU:CD1	0.54	2.82	21	1
1:B:82:VAL:CG1	1:B:84:ILE:HG13	0.54	2.33	24	7
1:B:38:LEU:HG	1:B:39:PRO:CD	0.54	2.33	6	2
1:A:55:LYS:O	1:A:79:PRO:HD2	0.54	2.02	15	25
1:A:60:ASP:O	1:A:61:GLN:HB2	0.54	2.03	21	27
1:A:38:LEU:HB2	1:A:59:TYR:CZ	0.54	2.38	26	4
1:A:32:VAL:HG13	1:A:33:LEU:N	0.54	2.18	2	12
1:B:25:ASP:OD2	2:B:100:DMP:C5	0.54	2.56	1	8
1:A:98:ASN:C	1:A:99:PHE:CD1	0.54	2.82	8	2
1:B:48:GLY:HA3	1:B:53:PHE:CE2	0.54	2.38	2	6
1:A:93:ILE:O	1:B:99:PHE:CB	0.54	2.56	25	3
1:A:99:PHE:CE2	1:B:24:LEU:HD13	0.54	2.38	20	3
1:A:89:LEU:O	1:A:92:GLN:OE1	0.54	2.26	17	1
1:B:86:GLY:C	1:B:90:LEU:CD1	0.54	2.76	17	1
1:B:15:ILE:CD1	1:B:75:VAL:CG1	0.54	2.86	18	2
1:B:4:THR:O	1:B:5:LEU:HB2	0.54	2.01	20	1
1:A:45:LYS:HE2	1:A:56:VAL:HG23	0.54	1.77	15	1
1:B:64:ILE:O	1:B:64:ILE:HG23	0.53	2.01	27	8
1:A:54:ILE:HG23	1:B:51:GLY:HA2	0.53	1.80	25	2
1:A:11:VAL:O	1:A:13:ILE:HG23	0.53	2.03	16	3
1:B:63:LEU:CD2	1:B:70:LYS:HG3	0.53	2.33	26	4
1:B:38:LEU:CD1	1:B:39:PRO:HD3	0.53	2.33	18	1
1:A:51:GLY:HA2	1:B:54:ILE:HG23	0.53	1.80	23	2
1:B:84:ILE:C	1:B:85:ILE:HD13	0.53	2.22	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:66:ILE:HG22	1:B:67:CYS:SG	0.53	2.43	7	1
1:B:33:LEU:C	1:B:80:THR:CG2	0.53	2.77	22	2
1:A:30:ASP:OD1	1:A:88:ASN:CB	0.53	2.57	8	6
1:A:25:ASP:OD2	2:B:100:DMP:C4	0.53	2.57	2	6
1:B:42:TRP:HB3	1:B:59:TYR:CD1	0.53	2.39	8	10
1:B:47:ILE:CG1	1:B:54:ILE:CG1	0.53	2.86	25	12
1:B:15:ILE:HG22	1:B:36:MET:CE	0.53	2.33	24	4
1:B:54:ILE:HD12	1:B:56:VAL:HG13	0.53	1.80	9	2
1:A:45:LYS:O	1:A:56:VAL:CG2	0.53	2.56	7	3
1:B:34:GLU:CG	1:B:80:THR:O	0.53	2.57	9	2
1:A:95:ALA:CB	1:B:99:PHE:CD1	0.53	2.91	24	2
1:B:32:VAL:O	1:B:33:LEU:CD1	0.53	2.54	7	13
1:A:80:THR:HG23	1:A:82:VAL:O	0.53	2.04	8	4
1:B:42:TRP:HB3	1:B:59:TYR:CE2	0.53	2.38	18	7
1:A:39:PRO:O	1:A:40:GLY:O	0.53	2.25	28	8
1:B:24:LEU:HD23	1:B:85:ILE:CG2	0.53	2.34	27	2
1:A:38:LEU:HD21	1:A:62:ILE:HG21	0.53	1.79	17	1
1:B:13:ILE:HD12	1:B:15:ILE:CG1	0.53	2.33	2	1
1:B:64:ILE:CD1	1:B:66:ILE:CD1	0.53	2.86	26	2
1:B:50:ILE:CG1	2:B:100:DMP:H62	0.53	2.34	23	21
1:B:38:LEU:HB2	1:B:59:TYR:CZ	0.53	2.39	20	8
1:B:80:THR:CG2	1:B:82:VAL:O	0.53	2.56	8	7
1:A:10:LEU:CD2	1:A:21:GLU:HB3	0.53	2.34	24	16
1:B:48:GLY:HA2	1:B:53:PHE:CD2	0.53	2.38	20	3
1:A:1:PRO:CD	1:B:99:PHE:O	0.53	2.56	6	1
1:A:14:LYS:HD2	1:A:19:LEU:HD11	0.53	1.81	20	1
1:B:90:LEU:N	1:B:90:LEU:CD1	0.53	2.71	20	2
1:B:38:LEU:HD13	1:B:62:ILE:CD1	0.53	2.34	15	1
1:B:10:LEU:CD2	1:B:21:GLU:CB	0.53	2.86	12	3
1:A:67:CYS:HB3	1:A:69:HIS:CD2	0.53	2.39	7	1
1:A:99:PHE:CZ	1:B:3:VAL:HG21	0.53	2.37	9	1
1:A:47:ILE:HG13	1:A:54:ILE:CG1	0.53	2.34	12	7
1:B:62:ILE:HB	1:B:75:VAL:HG23	0.53	1.81	18	12
1:A:45:LYS:CE	1:A:76:LEU:HD21	0.53	2.33	20	1
1:B:4:THR:O	1:B:5:LEU:CB	0.53	2.57	20	1
1:A:71:ALA:HB1	1:A:92:GLN:OE1	0.53	2.03	27	1
1:B:32:VAL:HG13	1:B:33:LEU:N	0.53	2.19	25	9
1:A:39:PRO:O	1:A:59:TYR:CD1	0.53	2.62	22	1
1:A:42:TRP:HB3	1:A:59:TYR:CE1	0.53	2.39	22	21
1:A:87:ARG:HA	1:A:90:LEU:HD23	0.53	1.79	7	1
1:A:19:LEU:O	1:A:20:LYS:CD	0.53	2.56	24	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:CB	1:A:39:PRO:HD2	0.53	2.34	19	5
1:A:11:VAL:CG2	1:A:13:ILE:CG2	0.53	2.87	9	1
1:A:24:LEU:CD2	1:A:85:ILE:HG21	0.53	2.34	10	1
1:B:19:LEU:O	1:B:20:LYS:CD	0.53	2.57	28	1
1:A:5:LEU:HD23	1:B:87:ARG:CB	0.53	2.33	18	1
1:B:10:LEU:CD2	1:B:21:GLU:HB3	0.53	2.34	28	11
1:B:88:ASN:O	1:B:92:GLN:NE2	0.53	2.42	13	2
1:B:82:VAL:CG1	1:B:84:ILE:HD11	0.53	2.33	21	4
1:B:34:GLU:CB	1:B:80:THR:O	0.53	2.56	21	2
1:A:22:ALA:HB1	1:A:85:ILE:CG1	0.53	2.33	28	2
1:A:45:LYS:CE	1:A:76:LEU:HD23	0.53	2.34	15	1
1:B:32:VAL:CG1	1:B:32:VAL:O	0.53	2.57	3	2
1:A:5:LEU:O	1:B:91:THR:CG2	0.53	2.56	3	1
1:A:50:ILE:O	1:B:50:ILE:O	0.52	2.28	12	28
1:A:29:ASP:OD2	1:B:8:ARG:CG	0.52	2.58	25	2
1:A:82:VAL:HG13	1:A:83:ASN:O	0.52	2.04	16	4
1:B:12:THR:HG22	1:B:19:LEU:CD2	0.52	2.30	11	2
1:A:4:THR:C	1:A:5:LEU:CD1	0.52	2.77	9	1
1:B:46:MET:SD	1:B:55:LYS:CE	0.52	2.97	10	1
1:B:26:THR:HG21	1:B:97:LEU:HD13	0.52	1.82	28	3
1:B:18:GLN:NE2	1:B:37:SER:O	0.52	2.43	28	1
1:B:43:LYS:O	1:B:58:GLN:CB	0.52	2.57	26	1
1:B:85:ILE:CG2	1:B:89:LEU:HB3	0.52	2.34	11	4
1:A:64:ILE:N	1:A:71:ALA:O	0.52	2.43	1	7
1:A:63:LEU:CD2	1:A:70:LYS:HG3	0.52	2.34	15	2
1:A:86:GLY:O	1:A:88:ASN:N	0.52	2.42	6	2
1:A:98:ASN:ND2	1:B:2:GLN:HG3	0.52	2.20	27	15
1:B:90:LEU:O	1:B:95:ALA:CB	0.52	2.57	13	2
1:B:42:TRP:CE3	1:B:57:ARG:HB3	0.52	2.39	18	5
1:B:13:ILE:HD12	1:B:64:ILE:HD11	0.52	1.82	14	1
1:A:85:ILE:HG23	1:A:89:LEU:HB3	0.52	1.79	5	2
1:A:38:LEU:HG	1:A:39:PRO:CD	0.52	2.34	6	2
1:A:88:ASN:O	1:A:92:GLN:NE2	0.52	2.42	27	2
1:A:38:LEU:CD2	1:A:62:ILE:HG21	0.52	2.35	17	1
1:A:76:LEU:HD12	1:A:76:LEU:H	0.52	1.65	1	3
1:B:85:ILE:HG23	1:B:89:LEU:CB	0.52	2.33	23	5
1:A:82:VAL:CG1	1:A:84:ILE:CD1	0.52	2.88	26	15
1:A:87:ARG:CZ	1:B:5:LEU:O	0.52	2.58	14	1
1:A:14:LYS:HE3	1:A:19:LEU:HD11	0.52	1.79	18	3
1:A:32:VAL:CG1	1:A:32:VAL:O	0.52	2.57	20	2
1:B:40:GLY:O	1:B:41:ARG:O	0.52	2.28	25	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ILE:HD12	1:A:79:PRO:HD2	0.52	1.82	8	1
1:B:86:GLY:O	1:B:90:LEU:HD13	0.52	2.05	21	4
1:B:90:LEU:CD2	1:B:90:LEU:N	0.52	2.73	10	1
1:B:58:GLN:NE2	1:B:74:THR:HG22	0.52	2.20	26	1
1:A:42:TRP:CE3	1:A:57:ARG:CD	0.52	2.93	20	1
1:B:13:ILE:CD1	1:B:15:ILE:HG13	0.52	2.34	15	1
1:A:9:PRO:HD3	1:B:87:ARG:NH2	0.52	2.19	21	1
1:A:4:THR:OG1	1:A:5:LEU:N	0.52	2.42	17	4
1:A:45:LYS:CG	1:A:46:MET:N	0.52	2.73	14	2
1:A:30:ASP:HB3	1:A:76:LEU:CD1	0.52	2.35	6	8
1:B:63:LEU:C	1:B:63:LEU:CD2	0.52	2.77	21	2
1:A:7:GLN:O	1:B:87:ARG:NE	0.52	2.42	3	2
1:A:13:ILE:HD12	1:A:15:ILE:HG13	0.52	1.79	15	4
1:A:97:LEU:HD13	1:B:5:LEU:HD23	0.52	1.82	5	1
1:B:63:LEU:HD22	1:B:63:LEU:C	0.52	2.24	28	1
1:A:31:THR:CG2	1:A:84:ILE:O	0.52	2.55	20	1
1:A:29:ASP:OD2	1:B:8:ARG:CZ	0.52	2.57	18	1
1:B:11:VAL:HG21	1:B:66:ILE:HG12	0.52	1.81	6	2
1:A:63:LEU:C	1:A:63:LEU:CD2	0.52	2.78	6	3
1:B:57:ARG:CD	1:B:77:VAL:O	0.52	2.58	18	1
1:A:87:ARG:NE	1:B:7:GLN:O	0.52	2.42	18	1
1:A:72:ILE:O	1:A:92:GLN:NE2	0.52	2.43	27	1
1:B:63:LEU:CA	1:B:72:ILE:HG12	0.52	2.35	5	8
1:B:15:ILE:HG22	1:B:36:MET:HE1	0.52	1.82	8	2
1:B:20:LYS:CB	1:B:83:ASN:ND2	0.52	2.73	17	6
1:A:31:THR:OG1	1:A:74:THR:O	0.52	2.28	13	1
1:A:15:ILE:HG22	1:A:36:MET:HE1	0.52	1.82	6	2
1:B:4:THR:OG1	1:B:5:LEU:N	0.52	2.42	24	4
1:A:89:LEU:HA	1:A:92:GLN:OE1	0.52	2.05	17	1
1:A:45:LYS:CE	1:A:56:VAL:HG23	0.52	2.35	15	1
1:B:15:ILE:HG21	1:B:62:ILE:CG2	0.52	2.34	15	1
1:B:89:LEU:HD13	1:B:92:GLN:HE21	0.52	1.65	25	1
1:A:11:VAL:HG23	1:A:11:VAL:O	0.52	2.02	23	7
1:A:32:VAL:HA	1:A:76:LEU:HB2	0.52	1.81	16	4
1:A:55:LYS:O	1:A:79:PRO:HD3	0.52	2.05	9	11
1:A:47:ILE:CG1	1:A:54:ILE:HG13	0.52	2.35	7	6
1:A:8:ARG:HB3	1:A:23:LEU:HD13	0.52	1.80	5	1
1:B:63:LEU:HD12	1:B:71:ALA:C	0.52	2.25	26	1
1:B:32:VAL:HG12	1:B:32:VAL:O	0.52	2.05	21	1
1:A:30:ASP:HA	1:A:88:ASN:OD1	0.52	2.04	17	8
1:A:31:THR:N	1:A:88:ASN:OD1	0.52	2.42	6	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ASP:HB3	1:A:84:ILE:HG22	0.52	1.81	23	3
1:B:21:GLU:O	1:B:83:ASN:HB2	0.52	2.04	7	9
1:A:11:VAL:HG21	1:A:66:ILE:HG12	0.52	1.82	16	1
1:B:21:GLU:N	1:B:21:GLU:OE1	0.52	2.43	9	1
1:B:82:VAL:CG1	1:B:83:ASN:O	0.52	2.58	3	1
1:B:63:LEU:CD2	1:B:63:LEU:C	0.51	2.77	12	1
1:A:50:ILE:HG13	2:B:100:DMP:H32	0.51	1.80	19	26
1:B:50:ILE:HG13	2:B:100:DMP:H62	0.51	1.83	18	28
1:A:5:LEU:CD1	1:B:95:ALA:O	0.51	2.58	11	1
1:A:34:GLU:N	1:A:80:THR:HG23	0.51	2.20	10	1
1:B:5:LEU:N	1:B:5:LEU:CD1	0.51	2.58	26	1
1:B:42:TRP:HB3	1:B:59:TYR:CZ	0.51	2.40	18	4
1:A:32:VAL:HG21	1:A:47:ILE:CD1	0.51	2.31	22	3
1:A:26:THR:HA	1:A:90:LEU:HD12	0.51	1.81	10	1
1:A:89:LEU:CA	1:A:92:GLN:OE1	0.51	2.58	17	1
1:A:64:ILE:HG23	1:A:64:ILE:O	0.51	2.05	12	4
1:A:82:VAL:HG12	1:A:84:ILE:HG13	0.51	1.83	5	4
1:B:47:ILE:CG1	1:B:54:ILE:HG12	0.51	2.36	15	4
1:B:15:ILE:CD1	1:B:33:LEU:CD2	0.51	2.89	5	2
1:A:26:THR:HG23	1:A:90:LEU:HD23	0.51	1.80	6	1
1:B:3:VAL:CG1	1:B:9:PRO:HB3	0.51	2.35	9	4
1:A:28:ALA:HB1	2:B:100:DMP:C27	0.51	2.36	5	2
1:A:25:ASP:OD1	1:B:25:ASP:OD1	0.51	2.29	5	23
1:A:82:VAL:HG12	1:A:84:ILE:CD1	0.51	2.36	23	14
1:A:87:ARG:O	1:A:91:THR:OG1	0.51	2.29	5	6
1:B:38:LEU:CB	1:B:39:PRO:HD2	0.51	2.36	8	3
1:A:54:ILE:CD1	1:A:54:ILE:C	0.51	2.78	11	1
1:A:42:TRP:HB3	1:A:59:TYR:CE2	0.51	2.41	19	2
1:B:42:TRP:CZ3	1:B:57:ARG:HD2	0.51	2.41	5	1
1:A:15:ILE:CD1	1:A:64:ILE:HD12	0.51	2.23	15	1
1:B:36:MET:SD	1:B:38:LEU:CD2	0.51	2.98	4	2
1:A:33:LEU:O	1:A:34:GLU:C	0.51	2.49	6	27
1:A:4:THR:CG2	1:B:96:THR:CG2	0.51	2.89	1	3
1:A:38:LEU:HB3	1:A:39:PRO:HD2	0.51	1.81	11	8
1:A:13:ILE:CG2	1:A:66:ILE:CG1	0.51	2.89	7	2
1:A:58:GLN:CG	1:A:74:THR:CG2	0.51	2.89	13	1
1:B:56:VAL:HA	1:B:77:VAL:O	0.51	2.05	20	7
1:A:99:PHE:CE2	1:B:1:PRO:HG2	0.51	2.41	17	4
1:A:47:ILE:CG1	1:A:54:ILE:HG12	0.51	2.36	28	1
1:B:38:LEU:HD12	1:B:59:TYR:CE2	0.51	2.40	15	1
1:A:20:LYS:HE2	1:A:20:LYS:N	0.51	2.20	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:ASP:O	1:B:61:GLN:CG	0.51	2.58	25	1
1:A:26:THR:CG2	1:A:90:LEU:HD13	0.51	2.33	3	1
1:B:60:ASP:O	1:B:61:GLN:HB2	0.51	2.05	7	26
1:A:2:GLN:HG3	1:B:98:ASN:ND2	0.51	2.21	2	21
1:B:87:ARG:O	1:B:91:THR:OG1	0.51	2.28	10	5
1:B:82:VAL:HG12	1:B:84:ILE:HG13	0.51	1.82	8	8
1:B:11:VAL:HG23	1:B:22:ALA:HB3	0.51	1.82	17	2
1:B:42:TRP:CD1	1:B:42:TRP:N	0.51	2.78	10	2
1:B:87:ARG:CA	1:B:90:LEU:CD1	0.51	2.88	17	1
1:B:86:GLY:C	1:B:90:LEU:HD12	0.51	2.26	17	1
1:B:13:ILE:HD12	1:B:15:ILE:HG12	0.51	1.81	2	1
1:A:99:PHE:HD2	1:B:95:ALA:HB2	0.51	1.66	27	11
1:B:87:ARG:HG2	1:B:87:ARG:NH1	0.51	2.19	16	1
1:B:34:GLU:N	1:B:80:THR:CG2	0.51	2.74	22	8
1:B:50:ILE:CD1	2:B:100:DMP:H26	0.51	2.36	14	3
1:B:15:ILE:O	1:B:36:MET:HE1	0.51	2.06	22	3
1:B:58:GLN:HG2	1:B:74:THR:HG22	0.51	1.83	22	1
1:B:93:ILE:HD11	1:B:95:ALA:HB2	0.51	1.82	9	2
1:B:33:LEU:C	1:B:80:THR:HG22	0.51	2.26	17	1
1:B:38:LEU:CB	1:B:59:TYR:CE1	0.51	2.93	4	2
1:A:30:ASP:OD1	1:A:88:ASN:ND2	0.51	2.43	27	1
1:A:61:GLN:HA	1:A:72:ILE:CG2	0.51	2.36	20	18
1:A:59:TYR:HB3	1:A:62:ILE:CG1	0.51	2.36	20	4
1:A:26:THR:HG23	1:A:87:ARG:NH2	0.51	2.21	23	1
1:B:15:ILE:HG22	1:B:38:LEU:HD13	0.51	1.82	16	1
1:B:38:LEU:HD23	1:B:39:PRO:CD	0.51	2.36	19	1
1:A:24:LEU:HD13	1:B:99:PHE:CE2	0.51	2.40	10	1
1:B:87:ARG:HD2	1:B:90:LEU:HD12	0.51	1.82	27	1
1:B:13:ILE:CD1	1:B:33:LEU:HD21	0.51	2.34	18	3
1:A:63:LEU:CD1	1:A:63:LEU:C	0.51	2.79	14	1
1:B:82:VAL:CG1	1:B:84:ILE:CD1	0.51	2.88	9	6
1:A:95:ALA:CB	1:B:5:LEU:HD12	0.51	2.34	6	1
1:B:38:LEU:CD2	1:B:39:PRO:HD2	0.51	2.36	19	3
1:B:22:ALA:CB	1:B:85:ILE:CD1	0.51	2.87	9	3
1:A:58:GLN:CD	1:A:74:THR:CG2	0.51	2.80	22	1
1:A:30:ASP:CA	1:A:88:ASN:OD1	0.51	2.58	17	2
1:A:82:VAL:HG11	1:A:84:ILE:HD11	0.51	1.83	20	1
1:B:76:LEU:HD12	1:B:76:LEU:H	0.51	1.63	15	1
1:A:90:LEU:HB3	1:A:95:ALA:HB3	0.51	1.83	25	2
1:A:22:ALA:CB	1:A:85:ILE:HD11	0.51	2.36	12	1
1:B:33:LEU:O	1:B:34:GLU:O	0.51	2.29	3	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:31:THR:HG22	1:B:33:LEU:HD13	0.51	1.80	8	2
1:A:66:ILE:O	1:A:67:CYS:C	0.51	2.49	21	6
1:A:65:GLU:OE1	1:A:70:LYS:N	0.51	2.44	18	1
1:A:58:GLN:HG3	1:A:74:THR:CG2	0.50	2.35	20	4
1:A:32:VAL:HG12	1:A:84:ILE:HB	0.50	1.81	8	3
1:A:72:ILE:HG22	1:A:73:GLY:N	0.50	2.21	20	5
1:B:39:PRO:O	1:B:40:GLY:O	0.50	2.29	13	9
1:A:64:ILE:O	1:A:64:ILE:HG23	0.50	2.05	18	4
1:B:72:ILE:CG2	1:B:73:GLY:N	0.50	2.74	18	8
1:A:8:ARG:NE	1:B:29:ASP:OD2	0.50	2.44	22	1
1:A:33:LEU:C	1:A:80:THR:CG2	0.50	2.80	10	1
1:A:13:ILE:HD13	1:A:22:ALA:HB2	0.50	1.82	20	1
1:A:6:TRP:CZ2	1:B:91:THR:O	0.50	2.65	12	1
1:A:54:ILE:HG12	1:B:50:ILE:CG2	0.50	2.37	11	7
1:B:22:ALA:HA	1:B:83:ASN:HB2	0.50	1.83	15	8
1:B:82:VAL:HG21	2:B:100:DMP:C33	0.50	2.36	15	1
1:A:62:ILE:HB	1:A:75:VAL:HG23	0.50	1.84	15	12
1:A:25:ASP:OD2	2:B:100:DMP:O5	0.50	2.29	17	9
1:B:58:GLN:HG2	1:B:74:THR:CG2	0.50	2.36	16	8
1:B:63:LEU:N	1:B:72:ILE:HG12	0.50	2.20	5	5
1:A:47:ILE:O	1:A:53:PHE:HA	0.50	2.06	8	13
1:A:15:ILE:CG2	1:A:36:MET:CE	0.50	2.88	8	4
1:B:10:LEU:HD23	1:B:22:ALA:O	0.50	2.06	1	3
1:B:45:LYS:HG3	1:B:56:VAL:CG2	0.50	2.37	1	2
1:A:58:GLN:OE1	1:A:74:THR:CG2	0.50	2.58	22	2
1:A:61:GLN:HA	1:A:72:ILE:HG23	0.50	1.84	25	6
1:A:96:THR:O	1:B:96:THR:O	0.50	2.30	9	5
1:A:21:GLU:O	1:A:83:ASN:HB2	0.50	2.07	13	8
1:B:89:LEU:CD1	1:B:92:GLN:OE1	0.50	2.59	13	2
1:B:62:ILE:HB	1:B:75:VAL:CG2	0.50	2.37	19	6
1:B:10:LEU:CD2	1:B:22:ALA:O	0.50	2.60	1	2
1:B:24:LEU:HD23	1:B:85:ILE:HG21	0.50	1.83	6	1
1:A:1:PRO:CG	1:A:67:CYS:SG	0.50	2.99	10	1
1:B:29:ASP:OD1	1:B:29:ASP:N	0.50	2.43	28	3
1:B:58:GLN:NE2	1:B:74:THR:CG2	0.50	2.75	26	1
1:A:8:ARG:HB3	1:A:23:LEU:HD11	0.50	1.83	4	1
1:B:30:ASP:OD1	1:B:88:ASN:CB	0.50	2.59	12	3
1:B:5:LEU:O	1:B:7:GLN:O	0.50	2.30	10	2
1:A:38:LEU:HD13	1:A:59:TYR:CG	0.50	2.42	24	2
1:B:34:GLU:N	1:B:80:THR:HG23	0.50	2.21	22	3
1:B:13:ILE:C	1:B:13:ILE:HD12	0.50	2.27	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:LEU:CG	1:B:39:PRO:CD	0.50	2.90	6	2
1:B:32:VAL:CG1	1:B:84:ILE:CG1	0.50	2.90	14	4
1:A:87:ARG:HA	1:A:90:LEU:HB2	0.50	1.82	25	2
1:B:85:ILE:HG22	1:B:90:LEU:HD23	0.50	1.83	10	1
1:A:47:ILE:HG12	1:A:54:ILE:CG1	0.50	2.37	28	1
1:A:32:VAL:HG23	1:A:76:LEU:CB	0.50	2.36	20	1
1:A:91:THR:HG22	1:B:5:LEU:CD2	0.50	2.37	27	1
1:A:81:PRO:O	1:A:82:VAL:CG2	0.50	2.57	17	3
1:B:42:TRP:N	1:B:42:TRP:CD1	0.50	2.80	12	3
1:A:59:TYR:O	1:A:62:ILE:CD1	0.50	2.59	9	2
1:A:5:LEU:HD23	1:A:5:LEU:O	0.50	2.06	13	1
1:A:31:THR:O	1:A:31:THR:HG22	0.50	2.07	5	4
1:A:86:GLY:O	1:A:90:LEU:HD13	0.50	2.05	6	1
1:B:57:ARG:N	1:B:57:ARG:HD2	0.50	2.22	6	1
1:A:2:GLN:HG2	1:B:98:ASN:ND2	0.50	2.22	22	3
1:A:24:LEU:HD12	1:B:99:PHE:CZ	0.50	2.42	28	1
1:A:33:LEU:O	1:A:34:GLU:O	0.50	2.29	20	18
1:A:29:ASP:OD1	1:A:29:ASP:N	0.50	2.45	23	2
1:A:87:ARG:HD2	1:B:7:GLN:O	0.50	2.07	16	1
1:B:31:THR:OG1	1:B:89:LEU:HG	0.50	2.07	16	1
1:A:84:ILE:C	1:A:85:ILE:HD12	0.50	2.27	11	4
1:A:26:THR:HA	1:A:90:LEU:CD1	0.50	2.37	14	6
1:A:91:THR:CG2	1:B:6:TRP:CE2	0.50	2.95	13	1
1:A:50:ILE:CG2	1:B:47:ILE:CD1	0.50	2.90	2	2
1:A:91:THR:HB	1:B:6:TRP:CZ3	0.50	2.42	22	2
1:B:58:GLN:CD	1:B:74:THR:CG2	0.50	2.80	22	1
1:A:5:LEU:CB	1:B:87:ARG:CZ	0.50	2.89	27	1
1:B:63:LEU:HD11	1:B:70:LYS:HG3	0.50	1.83	12	1
1:B:98:ASN:ND2	1:B:98:ASN:N	0.50	2.59	27	5
1:B:66:ILE:O	1:B:68:GLY:N	0.50	2.44	22	2
1:A:32:VAL:O	1:A:33:LEU:CD1	0.50	2.53	4	15
1:A:1:PRO:HD2	1:B:99:PHE:CD2	0.50	2.42	3	5
1:B:47:ILE:CG1	1:B:54:ILE:HG13	0.50	2.37	2	4
1:B:11:VAL:HG21	1:B:66:ILE:HG13	0.50	1.82	5	3
1:B:36:MET:N	1:B:77:VAL:CG1	0.50	2.75	26	1
1:B:62:ILE:HD12	1:B:62:ILE:N	0.50	2.22	4	1
1:A:95:ALA:CA	1:B:99:PHE:HB3	0.50	2.37	3	11
1:A:38:LEU:HB3	1:A:59:TYR:CD1	0.50	2.41	1	1
1:B:57:ARG:O	1:B:59:TYR:N	0.50	2.45	21	3
1:A:31:THR:HG22	1:A:33:LEU:HD12	0.50	1.84	10	2
1:A:15:ILE:CG2	1:A:38:LEU:HD21	0.50	2.36	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:63:LEU:HD11	1:B:70:LYS:CG	0.49	2.37	12	2
1:B:33:LEU:HD13	1:B:75:VAL:HG12	0.49	1.77	22	8
1:B:55:LYS:O	1:B:79:PRO:HD3	0.49	2.07	6	11
1:A:59:TYR:O	1:A:74:THR:HA	0.49	2.07	21	6
1:A:99:PHE:HB3	1:B:95:ALA:CA	0.49	2.37	4	11
1:B:38:LEU:HB3	1:B:59:TYR:CE2	0.49	2.42	6	3
1:A:51:GLY:N	1:B:54:ILE:HG23	0.49	2.21	28	5
1:A:95:ALA:HB3	1:B:5:LEU:CD1	0.49	2.36	6	1
1:B:59:TYR:HB3	1:B:62:ILE:CD1	0.49	2.36	20	4
1:A:97:LEU:HD13	1:B:5:LEU:CD2	0.49	2.37	5	1
1:A:1:PRO:HG2	1:B:99:PHE:CE2	0.49	2.41	3	2
1:B:81:PRO:C	1:B:82:VAL:CG2	0.49	2.80	15	1
1:A:59:TYR:HB3	1:A:62:ILE:CD1	0.49	2.37	25	6
1:B:32:VAL:C	1:B:33:LEU:HD12	0.49	2.26	22	3
1:A:63:LEU:CA	1:A:72:ILE:HG13	0.49	2.37	22	1
1:B:13:ILE:CD1	1:B:15:ILE:CD1	0.49	2.91	15	4
1:B:45:LYS:HE3	1:B:76:LEU:CD2	0.49	2.37	15	2
1:A:76:LEU:N	1:A:76:LEU:CD1	0.49	2.74	20	1
1:A:35:GLU:N	1:A:78:GLY:O	0.49	2.46	12	12
1:B:28:ALA:CB	2:B:100:DMP:H75	0.49	2.37	4	3
1:A:2:GLN:NE2	1:A:4:THR:HG21	0.49	2.22	12	1
1:A:29:ASP:HA	1:A:87:ARG:HG3	0.49	1.83	5	2
1:A:50:ILE:CD1	2:B:100:DMP:C71	0.49	2.90	13	1
1:B:57:ARG:N	1:B:57:ARG:CD	0.49	2.76	6	1
1:A:4:THR:O	1:B:87:ARG:NH1	0.49	2.45	24	1
1:A:59:TYR:O	1:A:74:THR:CG2	0.49	2.60	5	1
1:A:5:LEU:O	1:A:5:LEU:CD2	0.49	2.52	18	1
1:A:34:GLU:N	1:A:34:GLU:CD	0.49	2.66	12	1
1:A:10:LEU:HA	1:A:22:ALA:O	0.49	2.07	18	10
1:A:25:ASP:CB	1:B:27:GLY:HA3	0.49	2.37	9	3
1:A:38:LEU:CD1	1:A:77:VAL:CG2	0.49	2.89	24	1
1:B:29:ASP:OD1	1:B:87:ARG:NH2	0.49	2.46	9	2
1:A:73:GLY:HA3	1:A:89:LEU:CD2	0.49	2.37	17	2
1:A:13:ILE:CD1	1:A:15:ILE:HD12	0.49	2.38	27	2
1:A:54:ILE:CG2	1:B:51:GLY:HA2	0.49	2.37	27	9
1:B:34:GLU:O	1:B:77:VAL:HG13	0.49	2.07	12	1
1:B:33:LEU:O	1:B:34:GLU:C	0.49	2.50	26	23
1:B:63:LEU:HA	1:B:72:ILE:HG12	0.49	1.85	16	8
1:B:31:THR:HG23	1:B:85:ILE:HA	0.49	1.84	8	1
1:A:3:VAL:CG1	1:A:9:PRO:HB3	0.49	2.37	14	3
1:A:45:LYS:HD2	1:A:47:ILE:HG23	0.49	1.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:LEU:HD22	1:B:90:LEU:CD2	0.49	2.36	6	1
1:B:33:LEU:CD1	1:B:75:VAL:CG1	0.49	2.81	24	1
1:B:15:ILE:HD12	1:B:33:LEU:HD21	0.49	1.85	22	2
1:A:26:THR:CG2	1:B:9:PRO:HG3	0.49	2.37	25	1
1:A:6:TRP:CZ3	1:B:91:THR:HG21	0.49	2.43	11	2
1:B:46:MET:CE	1:B:53:PHE:HB3	0.49	2.37	10	1
1:A:99:PHE:CB	1:B:93:ILE:O	0.49	2.60	20	1
1:A:14:LYS:HD2	1:A:19:LEU:CG	0.49	2.38	4	2
1:A:22:ALA:HA	1:A:83:ASN:O	0.49	2.08	12	3
1:A:57:ARG:O	1:A:76:LEU:HA	0.49	2.07	17	6
1:B:15:ILE:CG2	1:B:36:MET:HE1	0.49	2.38	7	1
1:B:32:VAL:CG1	1:B:84:ILE:HG13	0.49	2.38	26	2
1:A:14:LYS:HD2	1:A:19:LEU:CD2	0.49	2.38	4	2
1:A:71:ALA:HB1	1:A:92:GLN:HE21	0.49	1.67	2	1
1:B:36:MET:N	1:B:77:VAL:HG11	0.49	2.22	26	1
1:B:11:VAL:CG2	1:B:66:ILE:HG13	0.49	2.37	27	1
1:A:99:PHE:HB3	1:B:95:ALA:N	0.49	2.22	24	5
1:A:99:PHE:CD2	1:B:1:PRO:HD2	0.49	2.43	17	3
1:A:5:LEU:CD2	1:A:5:LEU:O	0.49	2.53	9	1
1:A:42:TRP:CE3	1:A:57:ARG:HD3	0.49	2.43	20	2
1:A:3:VAL:HG12	1:A:9:PRO:HB3	0.49	1.84	20	1
1:A:26:THR:HG21	1:A:97:LEU:HD13	0.49	1.83	3	1
1:A:28:ALA:CB	2:B:100:DMP:H25	0.49	2.38	10	7
1:B:30:ASP:C	1:B:88:ASN:OD1	0.49	2.51	21	24
1:A:54:ILE:HG23	1:B:51:GLY:CA	0.49	2.38	23	3
1:A:11:VAL:CG2	1:A:11:VAL:O	0.49	2.61	9	5
1:A:85:ILE:O	1:A:85:ILE:HG22	0.49	2.07	18	5
1:B:57:ARG:HG2	1:B:77:VAL:O	0.49	2.07	19	3
1:B:89:LEU:N	1:B:89:LEU:HD23	0.49	2.23	16	1
1:B:15:ILE:CG1	1:B:64:ILE:HB	0.49	2.38	1	6
1:A:72:ILE:O	1:A:92:GLN:OE1	0.49	2.31	13	2
1:B:63:LEU:C	1:B:63:LEU:HD22	0.49	2.28	14	2
1:A:61:GLN:CD	1:A:61:GLN:N	0.49	2.66	14	1
1:A:38:LEU:CG	1:A:39:PRO:CD	0.49	2.91	6	2
1:B:64:ILE:N	1:B:71:ALA:O	0.49	2.46	28	5
1:A:38:LEU:CD2	1:A:62:ILE:CG2	0.49	2.91	17	1
1:B:38:LEU:HB3	1:B:59:TYR:CD1	0.49	2.42	4	1
1:B:25:ASP:OD2	2:B:100:DMP:O5	0.48	2.31	25	4
1:A:90:LEU:CD1	1:A:90:LEU:N	0.48	2.76	6	1
1:A:98:ASN:O	1:B:94:GLY:O	0.48	2.31	17	3
1:B:11:VAL:HG23	1:B:12:THR:N	0.48	2.22	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:45:LYS:NZ	1:B:76:LEU:CD2	0.48	2.74	15	1
1:A:25:ASP:OD1	2:B:100:DMP:O4	0.48	2.30	27	1
1:B:36:MET:SD	1:B:37:SER:O	0.48	2.71	5	5
1:B:13:ILE:CG2	1:B:66:ILE:HG13	0.48	2.38	9	3
1:A:42:TRP:CE3	1:A:57:ARG:HB3	0.48	2.43	9	3
1:B:22:ALA:HB1	1:B:85:ILE:CG1	0.48	2.37	15	2
1:A:5:LEU:HD13	1:A:6:TRP:N	0.48	2.22	18	1
1:A:54:ILE:HD11	1:A:56:VAL:HG13	0.48	1.84	6	2
1:B:22:ALA:HA	1:B:83:ASN:O	0.48	2.09	15	5
1:B:13:ILE:HA	1:B:65:GLU:O	0.48	2.09	19	9
1:B:63:LEU:C	1:B:63:LEU:CD1	0.48	2.81	16	1
1:A:63:LEU:N	1:A:72:ILE:CD1	0.48	2.75	7	5
1:B:35:GLU:HA	1:B:77:VAL:HG13	0.48	1.85	7	1
1:B:34:GLU:O	1:B:35:GLU:C	0.48	2.51	18	8
1:A:85:ILE:HD12	1:A:85:ILE:N	0.48	2.23	11	2
1:B:25:ASP:HB3	1:B:84:ILE:HG22	0.48	1.85	25	2
1:B:4:THR:O	1:B:5:LEU:CD1	0.48	2.55	5	1
1:A:99:PHE:HE2	1:B:24:LEU:HD13	0.48	1.66	20	1
1:B:47:ILE:O	1:B:53:PHE:HA	0.48	2.09	28	14
1:A:63:LEU:CA	1:A:72:ILE:HG12	0.48	2.39	11	3
1:A:25:ASP:OD1	2:B:100:DMP:O5	0.48	2.31	17	2
1:A:58:GLN:HG2	1:A:74:THR:CG2	0.48	2.38	9	3
1:B:5:LEU:C	1:B:5:LEU:CD2	0.48	2.82	1	1
1:A:6:TRP:CE3	1:A:6:TRP:HA	0.48	2.43	6	1
1:A:9:PRO:O	1:A:24:LEU:CG	0.48	2.61	2	1
1:A:34:GLU:N	1:A:80:THR:HG22	0.48	2.22	15	1
1:A:99:PHE:CB	1:B:93:ILE:CD1	0.48	2.88	15	1
1:A:87:ARG:NH1	1:B:9:PRO:HD3	0.48	2.22	3	1
1:A:11:VAL:CG2	1:A:13:ILE:HG23	0.48	2.37	7	2
1:A:62:ILE:HB	1:A:75:VAL:CG2	0.48	2.38	26	8
1:B:21:GLU:O	1:B:83:ASN:OD1	0.48	2.31	11	2
1:A:35:GLU:HA	1:A:77:VAL:CG1	0.48	2.38	22	10
1:B:38:LEU:CD1	1:B:77:VAL:CG2	0.48	2.92	5	3
1:B:42:TRP:HB3	1:B:59:TYR:CD2	0.48	2.44	19	4
1:A:25:ASP:HB2	1:A:84:ILE:CG2	0.48	2.37	14	2
1:A:38:LEU:HB3	1:A:59:TYR:CE2	0.48	2.43	19	1
1:B:6:TRP:O	1:B:7:GLN:OE1	0.48	2.32	19	1
1:A:91:THR:O	1:B:6:TRP:CZ2	0.48	2.66	24	1
1:A:11:VAL:CG1	1:A:24:LEU:HD11	0.48	2.39	2	1
1:B:13:ILE:HD13	1:B:15:ILE:CD1	0.48	2.39	23	2
1:A:34:GLU:OE1	1:A:83:ASN:ND2	0.48	2.46	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:O	1:B:99:PHE:OXT	0.48	2.32	1	2
1:B:10:LEU:HD23	1:B:21:GLU:C	0.48	2.29	20	1
1:A:9:PRO:CD	1:B:87:ARG:NH2	0.48	2.77	21	1
1:A:95:ALA:HA	1:B:98:ASN:O	0.48	2.08	7	18
1:B:38:LEU:O	1:B:59:TYR:CE2	0.48	2.66	16	1
1:B:34:GLU:HG2	1:B:35:GLU:N	0.48	2.22	3	2
1:A:58:GLN:HG2	1:A:60:ASP:OD1	0.48	2.08	10	1
1:A:10:LEU:CD2	1:A:21:GLU:CB	0.48	2.92	24	5
1:A:34:GLU:OE1	1:A:80:THR:O	0.48	2.31	23	1
1:B:26:THR:HA	1:B:87:ARG:NH2	0.48	2.23	16	1
1:A:6:TRP:CZ3	1:B:91:THR:HB	0.48	2.43	8	1
1:A:3:VAL:O	1:A:3:VAL:HG12	0.48	2.08	7	2
1:A:5:LEU:HD22	1:B:26:THR:HG23	0.48	1.86	11	1
1:A:66:ILE:HG22	1:A:66:ILE:O	0.48	2.08	1	1
1:B:88:ASN:O	1:B:89:LEU:HD22	0.48	2.09	18	2
1:B:38:LEU:CD2	1:B:62:ILE:CD1	0.48	2.91	6	1
1:B:38:LEU:CD2	1:B:62:ILE:HD12	0.48	2.36	6	1
1:A:30:ASP:OD2	1:A:88:ASN:OD1	0.48	2.31	5	1
1:B:63:LEU:CD2	1:B:70:LYS:HG2	0.48	2.39	10	1
1:A:85:ILE:CG2	1:A:89:LEU:HB3	0.48	2.38	17	2
1:A:60:ASP:OD1	1:A:60:ASP:N	0.48	2.46	26	1
1:B:60:ASP:C	1:B:61:GLN:CG	0.48	2.82	25	1
1:B:47:ILE:CD1	1:B:54:ILE:HD11	0.48	2.39	3	1
1:B:46:MET:CE	1:B:55:LYS:CG	0.48	2.91	4	1
1:B:85:ILE:HG23	1:B:89:LEU:HB2	0.48	1.85	23	3
1:B:25:ASP:OD2	2:B:100:DMP:O4	0.48	2.31	3	4
1:B:15:ILE:CG2	1:B:38:LEU:HD13	0.48	2.38	16	1
1:A:32:VAL:CG1	1:A:84:ILE:HG13	0.48	2.39	26	3
1:A:15:ILE:O	1:A:16:GLY:C	0.48	2.52	24	2
1:B:26:THR:CG2	1:B:87:ARG:HD3	0.48	2.39	13	2
1:A:82:VAL:CG1	1:A:84:ILE:HD13	0.48	2.39	1	1
1:A:21:GLU:O	1:A:83:ASN:CG	0.48	2.52	22	3
1:B:38:LEU:CD1	1:B:39:PRO:HD2	0.48	2.39	9	3
1:A:64:ILE:HD13	1:A:89:LEU:CD1	0.48	2.38	17	1
1:A:5:LEU:C	1:A:5:LEU:CD1	0.48	2.75	18	1
1:A:87:ARG:CD	1:B:7:GLN:C	0.48	2.82	18	1
1:B:54:ILE:CD1	1:B:56:VAL:HG13	0.48	2.38	4	1
1:A:34:GLU:HG2	1:A:80:THR:O	0.48	2.09	1	3
1:A:42:TRP:CB	1:A:58:GLN:O	0.48	2.62	16	1
1:A:13:ILE:CG2	1:A:66:ILE:HG13	0.48	2.36	5	3
1:B:22:ALA:HA	1:B:83:ASN:CB	0.48	2.38	26	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:THR:HA	1:B:90:LEU:CD2	0.48	2.39	14	2
1:B:56:VAL:HG21	1:B:76:LEU:HD23	0.48	1.86	1	1
1:A:60:ASP:OD1	1:A:74:THR:CG2	0.48	2.59	15	2
1:A:63:LEU:N	1:A:72:ILE:CG1	0.48	2.77	22	1
1:B:72:ILE:O	1:B:92:GLN:OE1	0.48	2.32	25	2
1:A:34:GLU:HG3	1:A:80:THR:O	0.47	2.09	8	4
1:A:15:ILE:HG23	1:A:64:ILE:HA	0.47	1.85	24	1
1:B:46:MET:CB	1:B:54:ILE:O	0.47	2.62	9	1
1:B:54:ILE:HD12	1:B:79:PRO:HD2	0.47	1.84	4	1
1:B:28:ALA:O	1:B:87:ARG:NH1	0.47	2.46	12	1
1:A:51:GLY:HA2	1:B:54:ILE:CG2	0.47	2.39	5	3
1:A:30:ASP:C	1:A:88:ASN:OD1	0.47	2.53	28	21
1:A:13:ILE:HA	1:A:65:GLU:O	0.47	2.09	1	12
1:A:47:ILE:HG12	1:A:54:ILE:CD1	0.47	2.38	11	1
1:A:28:ALA:O	1:A:86:GLY:CA	0.47	2.63	5	1
1:A:24:LEU:HD23	1:A:85:ILE:CB	0.47	2.37	26	1
1:B:26:THR:HG21	1:B:97:LEU:CD2	0.47	2.39	25	1
1:A:10:LEU:HG	1:A:22:ALA:O	0.47	2.10	9	5
1:B:22:ALA:CB	1:B:85:ILE:HD11	0.47	2.39	8	2
1:B:39:PRO:O	1:B:40:GLY:C	0.47	2.52	4	12
1:A:28:ALA:HB2	2:B:100:DMP:H25	0.47	1.87	11	2
1:A:15:ILE:HD11	1:A:64:ILE:HB	0.47	1.84	6	3
1:A:94:GLY:O	1:B:98:ASN:O	0.47	2.32	3	2
1:A:45:LYS:HE3	1:A:58:GLN:N	0.47	2.24	15	1
1:A:84:ILE:CD1	2:B:100:DMP:C62	0.47	2.85	12	1
1:A:36:MET:HG3	1:A:37:SER:N	0.47	2.24	16	2
1:B:36:MET:HG3	1:B:37:SER:N	0.47	2.25	14	3
1:A:3:VAL:CG1	1:A:5:LEU:HD23	0.47	2.26	24	1
1:B:32:VAL:CG2	1:B:76:LEU:HB2	0.47	2.39	3	4
1:A:58:GLN:CD	1:A:74:THR:HG22	0.47	2.29	22	1
1:B:15:ILE:HG22	1:B:36:MET:HE2	0.47	1.85	2	1
1:B:38:LEU:O	1:B:59:TYR:OH	0.47	2.30	2	1
1:B:3:VAL:HG11	1:B:9:PRO:CB	0.47	2.39	25	1
1:A:45:LYS:HB3	1:A:56:VAL:CG2	0.47	2.39	12	1
1:B:13:ILE:HB	1:B:64:ILE:CG1	0.47	2.40	26	6
1:A:97:LEU:HB3	1:A:99:PHE:CE2	0.47	2.44	2	3
1:B:54:ILE:HG13	1:B:54:ILE:O	0.47	2.10	13	2
1:A:39:PRO:O	1:A:59:TYR:OH	0.47	2.31	25	2
1:A:42:TRP:HB3	1:A:59:TYR:CD2	0.47	2.44	19	1
1:B:88:ASN:O	1:B:92:GLN:OE1	0.47	2.32	22	1
1:B:67:CYS:HB3	1:B:69:HIS:CD2	0.47	2.44	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:TRP:CZ3	1:A:57:ARG:HG2	0.47	2.45	25	2
1:B:81:PRO:O	1:B:82:VAL:HG22	0.47	2.09	15	1
1:A:67:CYS:O	1:A:69:HIS:CE1	0.47	2.68	3	1
1:B:15:ILE:HG23	1:B:38:LEU:HD21	0.47	1.85	13	2
1:B:15:ILE:O	1:B:17:GLY:N	0.47	2.47	8	2
1:B:86:GLY:O	1:B:87:ARG:C	0.47	2.53	22	7
1:A:4:THR:O	1:A:5:LEU:HB2	0.47	2.10	6	5
1:B:45:LYS:HG3	1:B:56:VAL:HG22	0.47	1.85	1	1
1:A:31:THR:CA	1:A:84:ILE:O	0.47	2.63	17	3
1:B:4:THR:C	1:B:5:LEU:CD1	0.47	2.76	1	2
1:A:62:ILE:O	1:A:64:ILE:N	0.47	2.48	22	1
1:A:5:LEU:C	1:A:5:LEU:HD22	0.47	2.22	18	2
1:A:80:THR:HG23	1:A:82:VAL:H	0.47	1.69	20	1
1:B:97:LEU:HB3	1:B:99:PHE:CZ	0.47	2.44	18	1
1:A:34:GLU:OE1	1:A:35:GLU:O	0.47	2.33	25	1
1:B:29:ASP:N	1:B:29:ASP:OD1	0.47	2.46	3	1
1:B:59:TYR:O	1:B:74:THR:HA	0.47	2.10	23	7
1:A:42:TRP:CA	1:A:58:GLN:O	0.47	2.62	16	1
1:A:22:ALA:HA	1:A:83:ASN:HB2	0.47	1.86	14	7
1:B:26:THR:HG22	1:B:26:THR:O	0.47	2.09	16	1
1:A:4:THR:CG2	1:B:96:THR:HB	0.47	2.39	7	1
1:B:34:GLU:OE1	1:B:80:THR:O	0.47	2.33	13	1
1:B:56:VAL:CG1	1:B:78:GLY:HA3	0.47	2.40	26	2
1:B:60:ASP:OD1	1:B:74:THR:CG2	0.47	2.58	17	3
1:A:50:ILE:CG2	1:B:54:ILE:HG12	0.47	2.40	19	6
1:A:63:LEU:CD2	1:A:70:LYS:HG2	0.47	2.36	15	2
1:A:69:HIS:HB3	1:A:93:ILE:HG22	0.47	1.86	21	2
1:B:33:LEU:CD1	1:B:75:VAL:HG13	0.47	2.32	15	1
1:B:26:THR:CG2	1:B:87:ARG:HD2	0.47	2.40	3	1
1:B:30:ASP:HA	1:B:88:ASN:OD1	0.47	2.10	8	8
1:A:23:LEU:O	1:A:24:LEU:C	0.47	2.53	23	21
1:B:47:ILE:HG13	1:B:54:ILE:CG1	0.47	2.38	8	4
1:A:15:ILE:HD12	1:A:75:VAL:CG1	0.47	2.35	6	2
1:A:24:LEU:CD2	1:A:24:LEU:N	0.47	2.77	25	1
1:A:27:GLY:CA	1:B:25:ASP:HA	0.47	2.40	17	5
1:B:34:GLU:HA	1:B:80:THR:HG23	0.47	1.86	16	1
1:B:42:TRP:CE3	1:B:57:ARG:CG	0.47	2.98	11	2
1:A:45:LYS:HB3	1:A:56:VAL:HG23	0.47	1.85	17	1
1:B:63:LEU:CD2	1:B:71:ALA:O	0.47	2.61	28	1
1:A:11:VAL:HG11	1:A:24:LEU:HD11	0.47	1.87	20	2
1:B:10:LEU:HA	1:B:22:ALA:O	0.47	2.10	1	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:LEU:HG	1:B:22:ALA:O	0.47	2.10	1	6
1:B:38:LEU:HD22	1:B:39:PRO:HD2	0.47	1.85	24	1
1:A:5:LEU:C	1:A:5:LEU:HD13	0.47	2.29	9	1
1:A:3:VAL:HG13	1:A:5:LEU:CD2	0.47	2.40	4	1
1:B:23:LEU:O	1:B:24:LEU:C	0.46	2.53	14	20
1:A:54:ILE:CD1	1:A:56:VAL:CG1	0.46	2.92	23	1
1:A:38:LEU:CB	1:A:59:TYR:CZ	0.46	2.97	16	1
1:A:19:LEU:O	1:A:20:LYS:HD2	0.46	2.10	14	3
1:B:59:TYR:HB3	1:B:62:ILE:HG13	0.46	1.87	14	4
1:B:63:LEU:CD2	1:B:72:ILE:HG13	0.46	2.40	24	1
1:A:46:MET:SD	1:A:54:ILE:O	0.46	2.73	22	2
1:B:42:TRP:CD2	1:B:57:ARG:HD3	0.46	2.45	10	1
1:A:98:ASN:O	1:B:95:ALA:HA	0.46	2.10	13	20
1:B:11:VAL:CG1	1:B:24:LEU:HD11	0.46	2.40	23	2
1:A:6:TRP:O	1:A:7:GLN:HG3	0.46	2.10	8	2
1:A:91:THR:O	1:B:6:TRP:CH2	0.46	2.68	8	2
1:A:72:ILE:CG2	1:A:73:GLY:N	0.46	2.78	26	9
1:B:72:ILE:HG22	1:B:73:GLY:N	0.46	2.24	10	4
1:B:42:TRP:CD1	1:B:59:TYR:CE2	0.46	3.03	19	2
1:A:62:ILE:CG2	1:A:75:VAL:HG21	0.46	2.38	24	1
1:A:62:ILE:C	1:A:72:ILE:HG12	0.46	2.31	22	1
1:B:2:GLN:OE1	1:B:4:THR:CG2	0.46	2.63	9	1
1:A:95:ALA:HB2	1:B:99:PHE:HD2	0.46	1.68	10	3
1:A:63:LEU:HA	1:A:71:ALA:O	0.46	2.09	15	2
1:A:82:VAL:HG12	1:A:83:ASN:N	0.46	2.25	17	1
1:A:64:ILE:HG21	1:A:89:LEU:CD1	0.46	2.40	21	2
1:B:25:ASP:OD2	1:B:28:ALA:CB	0.46	2.64	19	2
1:A:14:LYS:HA	1:A:18:GLN:O	0.46	2.10	6	12
1:B:57:ARG:HD3	1:B:57:ARG:N	0.46	2.25	19	1
1:B:34:GLU:OE1	1:B:35:GLU:O	0.46	2.34	10	1
1:A:7:GLN:O	1:A:8:ARG:C	0.46	2.54	18	2
1:B:38:LEU:CD1	1:B:62:ILE:HD12	0.46	2.40	26	1
1:A:38:LEU:HD12	1:A:39:PRO:CD	0.46	2.41	18	3
1:A:5:LEU:CD2	1:B:91:THR:CA	0.46	2.94	21	1
1:B:38:LEU:HD12	1:B:77:VAL:HG22	0.46	1.87	23	2
1:B:62:ILE:CG2	1:B:75:VAL:HG21	0.46	2.37	16	2
1:B:42:TRP:CG	1:B:59:TYR:CZ	0.46	3.03	14	3
1:A:64:ILE:HG12	1:A:66:ILE:CD1	0.46	2.40	7	4
1:B:47:ILE:HD11	1:B:54:ILE:CG1	0.46	2.41	7	1
1:B:45:LYS:HD3	1:B:76:LEU:HD23	0.46	1.87	14	1
1:A:58:GLN:OE1	1:A:58:GLN:O	0.46	2.34	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:GLY:C	1:B:23:LEU:HD21	0.46	2.30	2	1
1:B:5:LEU:H	1:B:5:LEU:HD22	0.46	1.68	25	1
1:A:33:LEU:HB2	1:A:75:VAL:HG12	0.46	1.88	25	5
1:B:97:LEU:HB3	1:B:99:PHE:CE2	0.46	2.45	11	2
1:B:85:ILE:HD12	1:B:85:ILE:N	0.46	2.26	1	3
1:B:50:ILE:CD1	2:B:100:DMP:C21	0.46	2.89	27	3
1:B:60:ASP:N	1:B:60:ASP:OD1	0.46	2.49	25	2
1:B:32:VAL:HG23	1:B:76:LEU:CB	0.46	2.40	22	1
1:B:21:GLU:N	1:B:21:GLU:CD	0.46	2.67	5	1
1:A:36:MET:HG2	1:A:77:VAL:HG11	0.46	1.88	2	1
1:A:47:ILE:CD1	1:B:50:ILE:CG2	0.46	2.91	25	1
1:A:69:HIS:O	1:A:70:LYS:C	0.46	2.52	17	4
1:A:39:PRO:O	1:A:40:GLY:C	0.46	2.52	26	5
1:A:36:MET:CG	1:A:37:SER:N	0.46	2.78	12	3
1:A:87:ARG:O	1:A:88:ASN:C	0.46	2.53	13	13
1:A:45:LYS:HG2	1:A:76:LEU:HD23	0.46	1.86	7	1
1:A:63:LEU:HA	1:A:72:ILE:HG12	0.46	1.87	11	5
1:A:63:LEU:N	1:A:72:ILE:HG12	0.46	2.25	22	2
1:A:56:VAL:HG12	1:A:78:GLY:N	0.46	2.24	20	1
1:A:26:THR:HG22	1:A:87:ARG:HH12	0.46	1.69	18	1
1:A:45:LYS:CB	1:A:56:VAL:HG23	0.46	2.38	12	2
1:A:34:GLU:O	1:A:35:GLU:C	0.46	2.54	18	7
1:B:73:GLY:HA3	1:B:89:LEU:CD2	0.46	2.41	9	7
1:B:63:LEU:HD23	1:B:72:ILE:HG12	0.46	1.88	9	4
1:A:25:ASP:OD2	2:B:100:DMP:H4	0.46	2.10	13	2
1:B:45:LYS:HG2	1:B:56:VAL:CG2	0.46	2.40	28	2
1:A:54:ILE:HG22	1:B:51:GLY:HA2	0.46	1.88	14	1
1:A:1:PRO:HD2	1:B:99:PHE:O	0.46	2.10	28	2
1:B:57:ARG:CG	1:B:77:VAL:HB	0.46	2.41	19	1
1:B:68:GLY:C	1:B:69:HIS:CG	0.46	2.89	22	1
1:A:32:VAL:HB	2:B:100:DMP:O27	0.46	2.10	5	1
1:B:14:LYS:CG	1:B:19:LEU:HG	0.46	2.40	10	1
1:A:85:ILE:CG2	1:A:89:LEU:CB	0.46	2.93	3	3
1:A:65:GLU:OE2	1:A:69:HIS:N	0.46	2.49	28	1
1:A:97:LEU:HB3	1:A:99:PHE:CZ	0.46	2.46	2	1
1:B:40:GLY:O	1:B:41:ARG:HG3	0.46	2.10	18	2
1:B:13:ILE:HD12	1:B:15:ILE:CD1	0.46	2.41	4	1
1:B:25:ASP:OD2	2:B:100:DMP:H5	0.46	2.10	3	4
1:B:34:GLU:HG3	1:B:80:THR:O	0.46	2.10	9	3
1:B:11:VAL:O	1:B:13:ILE:HG23	0.46	2.11	19	4
1:B:57:ARG:O	1:B:76:LEU:HA	0.46	2.11	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:LEU:O	1:A:20:LYS:HD3	0.46	2.11	27	2
1:B:65:GLU:OE2	1:B:68:GLY:N	0.46	2.49	24	1
1:B:32:VAL:HG21	1:B:47:ILE:CD1	0.46	2.40	22	1
1:B:32:VAL:HG11	1:B:84:ILE:HD12	0.46	1.87	22	1
1:A:27:GLY:CA	1:B:23:LEU:HD21	0.46	2.40	4	2
1:B:40:GLY:O	1:B:41:ARG:HB2	0.46	2.10	22	6
1:A:8:ARG:NE	1:B:29:ASP:OD1	0.46	2.49	26	1
1:B:36:MET:SD	1:B:38:LEU:HD21	0.46	2.51	15	1
1:A:9:PRO:HB2	1:A:24:LEU:HB2	0.46	1.88	3	1
1:A:9:PRO:CB	1:A:24:LEU:HB2	0.46	2.40	3	1
1:A:55:LYS:O	1:A:78:GLY:HA3	0.46	2.11	25	6
1:A:6:TRP:CH2	1:B:91:THR:O	0.46	2.69	12	1
1:B:85:ILE:CG2	1:B:89:LEU:HB2	0.46	2.41	23	1
1:A:15:ILE:HD12	1:A:33:LEU:HD21	0.46	1.88	1	5
1:B:30:ASP:HB2	1:B:76:LEU:CD1	0.46	2.41	8	1
1:A:46:MET:SD	1:A:54:ILE:C	0.46	2.94	13	2
1:A:95:ALA:N	1:B:99:PHE:HB3	0.46	2.26	7	6
1:B:62:ILE:O	1:B:72:ILE:HA	0.46	2.11	25	3
1:B:58:GLN:NE2	1:B:60:ASP:OD1	0.46	2.49	14	2
1:B:59:TYR:O	1:B:62:ILE:HG12	0.46	2.11	19	1
1:A:99:PHE:HB2	1:B:93:ILE:O	0.46	2.11	20	3
1:B:43:LYS:O	1:B:58:GLN:N	0.46	2.49	19	1
1:A:2:GLN:HG2	1:A:3:VAL:N	0.46	2.26	22	2
1:A:25:ASP:OD2	1:A:28:ALA:CB	0.46	2.64	5	1
1:A:41:ARG:N	1:A:41:ARG:HD3	0.46	2.26	10	1
1:B:5:LEU:CD1	1:B:9:PRO:HA	0.46	2.38	10	1
1:A:45:LYS:NZ	1:A:76:LEU:HD23	0.46	2.26	20	1
1:A:14:LYS:CE	1:A:19:LEU:HD11	0.46	2.41	18	1
1:A:85:ILE:CG2	1:A:85:ILE:O	0.46	2.64	16	1
1:B:38:LEU:CG	1:B:39:PRO:HD2	0.46	2.40	6	2
1:B:10:LEU:CG	1:B:22:ALA:O	0.46	2.64	1	1
1:A:87:ARG:CZ	1:B:9:PRO:HD2	0.46	2.41	17	1
1:A:91:THR:CG2	1:B:6:TRP:HB3	0.46	2.40	17	1
1:B:18:GLN:HB2	1:B:36:MET:HE1	0.46	1.88	26	1
1:A:50:ILE:HD11	1:B:84:ILE:HD11	0.46	1.85	15	1
1:B:90:LEU:CD2	1:B:95:ALA:CB	0.46	2.94	18	1
1:A:7:GLN:HA	1:B:87:ARG:NH1	0.45	2.26	23	1
1:A:42:TRP:HA	1:A:58:GLN:O	0.45	2.11	16	1
1:A:13:ILE:HB	1:A:64:ILE:CG1	0.45	2.41	4	3
1:B:11:VAL:CG2	1:B:13:ILE:CG2	0.45	2.94	5	3
1:B:46:MET:CE	1:B:53:PHE:CB	0.45	2.94	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ALA:CB	1:A:92:GLN:NE2	0.45	2.78	17	1
1:B:63:LEU:HD23	1:B:63:LEU:C	0.45	2.31	21	1
1:B:38:LEU:HG	1:B:62:ILE:CD1	0.45	2.41	8	1
1:A:42:TRP:CE3	1:A:57:ARG:HG2	0.45	2.46	26	2
1:A:91:THR:CG2	1:B:5:LEU:CD2	0.45	2.94	1	1
1:B:11:VAL:HG23	1:B:11:VAL:O	0.45	2.11	6	2
1:A:12:THR:CG2	1:A:19:LEU:CD2	0.45	2.94	9	1
1:A:54:ILE:HG13	1:A:54:ILE:O	0.45	2.11	18	2
1:B:34:GLU:HG3	1:B:35:GLU:N	0.45	2.25	18	1
1:B:46:MET:HG2	1:B:55:LYS:CG	0.45	2.40	9	3
1:B:6:TRP:O	1:B:7:GLN:HG3	0.45	2.11	16	2
1:B:64:ILE:CG2	1:B:89:LEU:HD13	0.45	2.40	16	1
1:A:6:TRP:O	1:A:7:GLN:CG	0.45	2.65	8	2
1:B:63:LEU:HA	1:B:71:ALA:O	0.45	2.11	11	3
1:A:54:ILE:O	1:A:54:ILE:HG13	0.45	2.11	13	1
1:A:36:MET:SD	1:A:37:SER:O	0.45	2.75	13	2
1:B:41:ARG:C	1:B:42:TRP:CD1	0.45	2.89	10	1
1:A:25:ASP:O	1:A:86:GLY:HA2	0.45	2.11	28	1
1:B:14:LYS:HE3	1:B:19:LEU:CD1	0.45	2.40	26	1
1:B:69:HIS:CB	1:B:93:ILE:HG22	0.45	2.35	25	1
1:B:59:TYR:C	1:B:62:ILE:CD1	0.45	2.84	4	1
1:B:87:ARG:O	1:B:89:LEU:N	0.45	2.50	27	1
1:A:32:VAL:CG2	1:A:76:LEU:HB2	0.45	2.41	2	6
1:A:93:ILE:O	1:B:99:PHE:HB2	0.45	2.10	25	5
1:B:59:TYR:O	1:B:74:THR:CG2	0.45	2.64	8	1
1:A:15:ILE:CG1	1:A:64:ILE:HB	0.45	2.41	4	4
1:B:31:THR:O	1:B:76:LEU:HD12	0.45	2.10	7	2
1:B:85:ILE:O	1:B:85:ILE:HG22	0.45	2.12	13	4
1:B:28:ALA:HB2	2:B:100:DMP:H75	0.45	1.87	4	2
1:A:6:TRP:CE3	1:B:91:THR:CB	0.45	2.99	13	1
1:A:6:TRP:HA	1:B:91:THR:HG21	0.45	1.88	13	1
1:B:87:ARG:HA	1:B:90:LEU:HB2	0.45	1.88	14	3
1:B:39:PRO:O	1:B:59:TYR:OH	0.45	2.33	21	2
1:A:45:LYS:HE2	1:A:76:LEU:CD2	0.45	2.40	17	2
1:A:59:TYR:HB3	1:A:62:ILE:HG13	0.45	1.89	18	3
1:B:14:LYS:HE3	1:B:19:LEU:HD11	0.45	1.88	2	2
1:B:13:ILE:HD12	1:B:64:ILE:CD1	0.45	2.41	14	1
1:B:5:LEU:HD22	1:B:6:TRP:H	0.45	1.71	27	2
1:A:86:GLY:O	1:A:87:ARG:C	0.45	2.54	6	2
1:A:38:LEU:CG	1:A:39:PRO:HD2	0.45	2.40	6	4
1:A:87:ARG:CZ	1:A:87:ARG:HB2	0.45	2.41	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:VAL:O	1:A:4:THR:C	0.45	2.53	9	1
1:A:68:GLY:O	1:A:69:HIS:HB2	0.45	2.11	17	1
1:B:86:GLY:O	1:B:90:LEU:HD12	0.45	2.11	17	1
1:A:63:LEU:HD11	1:A:70:LYS:CD	0.45	2.40	4	1
1:B:62:ILE:CG1	1:B:75:VAL:HG23	0.45	2.41	13	1
1:A:82:VAL:HG12	1:A:83:ASN:O	0.45	2.12	14	1
1:A:22:ALA:CB	1:A:85:ILE:HD13	0.45	2.28	14	1
1:A:91:THR:HG23	1:B:5:LEU:CG	0.45	2.41	1	1
1:A:30:ASP:CG	1:A:88:ASN:OD1	0.45	2.55	17	1
1:B:36:MET:CE	1:B:38:LEU:HD21	0.45	2.41	15	1
1:A:26:THR:HA	1:A:90:LEU:CD2	0.45	2.42	25	1
1:B:19:LEU:O	1:B:20:LYS:HG2	0.45	2.11	12	1
1:B:13:ILE:HD12	1:B:13:ILE:O	0.45	2.11	23	1
1:B:58:GLN:OE1	1:B:60:ASP:OD2	0.45	2.34	23	1
1:B:33:LEU:CD2	1:B:83:ASN:OD1	0.45	2.64	7	2
1:A:86:GLY:C	1:A:90:LEU:HD22	0.45	2.31	7	1
1:A:83:ASN:C	1:A:84:ILE:CG1	0.45	2.85	14	1
1:A:32:VAL:HG12	1:A:84:ILE:CB	0.45	2.41	19	3
1:A:89:LEU:O	1:A:92:GLN:CD	0.45	2.55	17	1
1:B:97:LEU:HD23	1:B:99:PHE:CE1	0.45	2.46	28	1
1:A:69:HIS:HB3	1:A:93:ILE:CG2	0.45	2.41	21	1
1:A:93:ILE:O	1:B:99:PHE:O	0.45	2.35	25	1
1:A:98:ASN:N	1:A:98:ASN:ND2	0.45	2.64	12	3
1:B:59:TYR:HB3	1:B:62:ILE:CG1	0.45	2.42	14	7
1:A:26:THR:OG1	1:B:26:THR:OG1	0.45	2.32	18	2
1:B:46:MET:CG	1:B:55:LYS:HG3	0.45	2.41	7	4
1:A:47:ILE:HD11	1:A:54:ILE:HG12	0.45	1.88	13	1
1:B:14:LYS:HG3	1:B:19:LEU:CD2	0.45	2.42	20	3
1:A:32:VAL:C	1:A:33:LEU:HD12	0.45	2.30	5	2
1:B:36:MET:O	1:B:77:VAL:HG11	0.45	2.12	5	1
1:B:42:TRP:CE3	1:B:57:ARG:HD2	0.45	2.47	5	1
1:B:36:MET:CG	1:B:38:LEU:HD23	0.45	2.41	9	1
1:A:13:ILE:O	1:A:19:LEU:CD2	0.45	2.56	17	1
1:A:46:MET:HB3	1:A:54:ILE:O	0.45	2.12	20	1
1:B:88:ASN:C	1:B:89:LEU:HD22	0.45	2.31	18	1
1:A:47:ILE:HG13	1:A:54:ILE:HG13	0.45	1.89	22	5
1:A:3:VAL:CG1	1:A:3:VAL:O	0.45	2.64	12	1
1:A:40:GLY:O	1:A:41:ARG:HG3	0.45	2.12	12	1
1:A:47:ILE:O	1:A:53:PHE:CA	0.45	2.64	8	2
1:A:38:LEU:O	1:A:59:TYR:CE1	0.45	2.70	13	1
1:A:95:ALA:O	1:B:5:LEU:HG	0.45	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:CD2	1:B:97:LEU:HD13	0.45	2.41	6	1
1:B:6:TRP:O	1:B:7:GLN:HG2	0.45	2.12	19	2
1:B:97:LEU:HB3	1:B:99:PHE:CE1	0.45	2.47	26	4
1:B:82:VAL:CG2	2:B:100:DMP:C33	0.45	2.94	15	1
1:A:5:LEU:HB3	1:B:87:ARG:HG2	0.45	1.88	3	1
1:A:21:GLU:N	1:A:21:GLU:CD	0.45	2.69	12	1
1:B:89:LEU:HD13	1:B:92:GLN:CD	0.45	2.32	23	1
1:A:25:ASP:OD1	1:B:27:GLY:HA3	0.45	2.12	16	1
1:A:34:GLU:CA	1:A:80:THR:CG2	0.45	2.95	16	5
1:B:2:GLN:HG2	1:B:3:VAL:N	0.45	2.26	14	7
1:B:55:LYS:O	1:B:78:GLY:HA3	0.45	2.10	1	6
1:A:29:ASP:N	1:A:29:ASP:OD1	0.45	2.49	8	1
1:A:38:LEU:CD1	1:A:62:ILE:HD12	0.45	2.41	13	1
1:A:15:ILE:CD1	1:A:75:VAL:CG1	0.45	2.95	19	2
1:A:15:ILE:HD13	1:A:36:MET:CE	0.45	2.42	24	1
1:A:83:ASN:O	1:A:84:ILE:HG13	0.45	2.11	20	1
1:B:13:ILE:HG21	1:B:64:ILE:HD11	0.44	1.89	12	1
1:B:33:LEU:N	1:B:76:LEU:O	0.44	2.50	12	3
1:B:87:ARG:O	1:B:88:ASN:C	0.44	2.55	27	7
1:A:56:VAL:HA	1:A:77:VAL:O	0.44	2.12	20	7
1:B:58:GLN:CG	1:B:74:THR:HG21	0.44	2.41	16	1
1:A:51:GLY:CA	1:B:54:ILE:CG2	0.44	2.95	5	1
1:A:4:THR:O	1:A:5:LEU:CD1	0.44	2.61	9	1
1:A:5:LEU:HD13	1:B:90:LEU:HB3	0.44	1.90	10	1
1:B:45:LYS:HG3	1:B:45:LYS:O	0.44	2.12	2	1
1:B:89:LEU:HD22	1:B:92:GLN:NE2	0.44	2.27	21	1
1:A:65:GLU:OE1	1:A:70:LYS:HA	0.44	2.12	18	1
1:B:9:PRO:CB	1:B:24:LEU:HD12	0.44	2.41	18	1
1:B:54:ILE:HD11	1:B:56:VAL:CG1	0.44	2.41	4	1
1:B:5:LEU:C	1:B:7:GLN:N	0.44	2.71	10	4
1:A:98:ASN:ND2	1:A:98:ASN:N	0.44	2.65	16	3
1:A:11:VAL:O	1:A:11:VAL:HG23	0.44	2.12	5	2
1:A:62:ILE:HG21	1:A:75:VAL:CG2	0.44	2.41	24	1
1:B:63:LEU:HA	1:B:72:ILE:CG1	0.44	2.42	5	1
1:A:38:LEU:CD2	1:A:62:ILE:HD12	0.44	2.40	17	1
1:A:34:GLU:CG	1:A:35:GLU:N	0.44	2.80	2	1
1:A:36:MET:SD	1:A:37:SER:N	0.44	2.91	25	2
1:A:26:THR:HG22	1:A:87:ARG:NH2	0.44	2.26	3	1
1:A:5:LEU:HD12	1:B:87:ARG:CD	0.44	2.41	27	1
1:B:31:THR:CA	1:B:84:ILE:O	0.44	2.65	14	3
1:A:38:LEU:HD21	1:A:62:ILE:CD1	0.44	2.43	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:THR:CG2	1:A:82:VAL:O	0.44	2.65	8	3
1:A:99:PHE:OXT	1:B:1:PRO:CD	0.44	2.65	8	2
1:A:15:ILE:O	1:A:36:MET:HE1	0.44	2.12	11	1
1:B:62:ILE:HG13	1:B:75:VAL:HG23	0.44	1.89	13	1
1:B:59:TYR:CD1	1:B:77:VAL:CG2	0.44	3.00	14	1
1:A:46:MET:CG	1:A:55:LYS:HG2	0.44	2.42	1	2
1:B:89:LEU:CD1	1:B:92:GLN:NE2	0.44	2.79	22	1
1:A:87:ARG:NH1	1:A:90:LEU:CB	0.44	2.80	22	1
1:A:1:PRO:HG2	1:A:67:CYS:SG	0.44	2.52	10	1
1:B:26:THR:HG21	1:B:97:LEU:CD1	0.44	2.42	10	1
1:A:46:MET:CG	1:A:55:LYS:HG3	0.44	2.42	2	1
1:B:18:GLN:HB2	1:B:36:MET:CE	0.44	2.41	26	1
1:A:8:ARG:NH1	1:A:8:ARG:HG2	0.44	2.28	26	1
1:A:82:VAL:HG13	1:A:84:ILE:CG1	0.44	2.41	20	1
1:B:30:ASP:HA	1:B:88:ASN:CG	0.44	2.33	15	2
1:A:61:GLN:OE1	1:A:61:GLN:CA	0.44	2.66	27	1
1:A:13:ILE:HG13	1:A:13:ILE:O	0.44	2.12	23	2
1:A:97:LEU:HB3	1:A:99:PHE:CE1	0.44	2.48	14	2
1:A:6:TRP:CE2	1:B:91:THR:HB	0.44	2.47	13	1
1:A:82:VAL:HG12	1:A:84:ILE:HG12	0.44	1.86	14	1
1:B:39:PRO:O	1:B:59:TYR:CZ	0.44	2.70	24	1
1:B:36:MET:HG3	1:B:38:LEU:CD2	0.44	2.43	9	1
1:A:14:LYS:O	1:A:63:LEU:O	0.44	2.35	9	1
1:A:87:ARG:NH2	1:B:9:PRO:HD2	0.44	2.27	17	1
1:B:7:GLN:O	1:B:9:PRO:HD3	0.44	2.11	17	1
1:B:43:LYS:O	1:B:58:GLN:HB3	0.44	2.11	26	1
1:B:89:LEU:HD22	1:B:92:GLN:HE22	0.44	1.72	21	1
1:B:30:ASP:HB3	1:B:76:LEU:HD12	0.44	1.89	4	1
1:B:6:TRP:O	1:B:7:GLN:CG	0.44	2.66	4	1
1:A:15:ILE:CG1	1:A:64:ILE:HA	0.44	2.42	27	1
1:A:90:LEU:HD22	1:A:95:ALA:CB	0.44	2.42	27	1
1:A:5:LEU:HB3	1:B:87:ARG:NE	0.44	2.28	27	1
1:B:16:GLY:HA3	1:B:38:LEU:CD1	0.44	2.42	16	2
1:A:47:ILE:O	1:A:53:PHE:HB3	0.44	2.13	8	3
1:A:5:LEU:HD22	1:B:26:THR:HG21	0.44	1.90	6	1
1:A:48:GLY:HA3	1:A:53:PHE:CD1	0.44	2.47	6	1
1:A:86:GLY:O	1:A:90:LEU:HG	0.44	2.13	19	3
1:A:62:ILE:HD12	1:A:62:ILE:N	0.44	2.28	9	1
1:B:25:ASP:HB2	1:B:84:ILE:CG2	0.44	2.42	9	1
1:B:38:LEU:HG	1:B:59:TYR:CG	0.44	2.48	26	1
1:A:5:LEU:CD2	1:B:87:ARG:HB3	0.44	2.39	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HD11	1:A:9:PRO:CD	0.44	2.43	27	1
1:B:26:THR:HA	1:B:90:LEU:CD1	0.44	2.42	12	2
1:A:15:ILE:CG2	1:A:36:MET:HE1	0.44	2.42	8	1
1:B:45:LYS:CG	1:B:56:VAL:CG2	0.44	2.96	14	2
1:A:64:ILE:CD1	1:A:66:ILE:CD1	0.44	2.89	5	2
1:A:82:VAL:CG1	1:A:84:ILE:HG12	0.44	2.43	5	1
1:A:84:ILE:HD12	1:B:50:ILE:HD11	0.44	1.90	5	1
1:A:45:LYS:CD	1:A:58:GLN:HB2	0.44	2.43	5	1
1:B:34:GLU:HA	1:B:80:THR:O	0.44	2.12	2	1
1:B:34:GLU:HG2	1:B:82:VAL:N	0.44	2.27	2	1
1:A:56:VAL:CG1	1:A:78:GLY:HA3	0.44	2.39	20	1
1:A:18:GLN:NE2	1:A:18:GLN:HA	0.44	2.28	18	1
1:B:11:VAL:CG2	1:B:12:THR:N	0.44	2.80	3	1
1:A:63:LEU:HD11	1:A:71:ALA:N	0.44	2.26	23	2
1:B:16:GLY:CA	1:B:38:LEU:CD1	0.44	2.96	16	1
1:B:88:ASN:OD1	1:B:89:LEU:N	0.44	2.51	16	1
1:B:31:THR:O	1:B:75:VAL:HA	0.44	2.13	24	3
1:B:15:ILE:HD13	1:B:33:LEU:HD22	0.44	1.89	8	1
1:B:59:TYR:CE1	1:B:77:VAL:CG2	0.44	3.01	14	1
1:B:47:ILE:O	1:B:53:PHE:HB3	0.44	2.13	28	2
1:B:8:ARG:HB3	1:B:23:LEU:HD12	0.44	1.90	22	1
1:B:4:THR:C	1:B:5:LEU:HG	0.44	2.33	5	1
1:A:63:LEU:CD1	1:A:72:ILE:HG13	0.44	2.42	15	1
1:B:8:ARG:HB3	1:B:23:LEU:CD1	0.44	2.43	18	3
1:A:89:LEU:O	1:A:93:ILE:HG12	0.44	2.12	25	2
1:B:14:LYS:HD3	1:B:19:LEU:HD21	0.44	1.89	27	1
1:B:9:PRO:O	1:B:24:LEU:HG	0.44	2.13	4	3
1:B:14:LYS:HA	1:B:18:GLN:O	0.44	2.12	15	7
1:A:48:GLY:HA2	1:A:53:PHE:CD2	0.44	2.47	13	2
1:B:65:GLU:HA	1:B:69:HIS:O	0.44	2.12	7	1
1:B:66:ILE:O	1:B:67:CYS:HB2	0.44	2.13	6	5
1:B:6:TRP:CD1	1:B:6:TRP:N	0.44	2.86	13	4
1:A:91:THR:HG21	1:B:6:TRP:CD1	0.44	2.46	13	1
1:A:57:ARG:HG3	1:A:77:VAL:O	0.44	2.12	1	1
1:A:30:ASP:OD1	1:A:88:ASN:CG	0.44	2.56	19	1
1:A:15:ILE:HG23	1:A:64:ILE:CA	0.44	2.42	24	1
1:B:38:LEU:CD2	1:B:39:PRO:CD	0.44	2.95	24	1
1:B:15:ILE:CD1	1:B:75:VAL:HG21	0.44	2.37	18	2
1:A:85:ILE:N	1:A:85:ILE:HD12	0.44	2.28	22	1
1:A:58:GLN:OE1	1:A:76:LEU:HD21	0.44	2.13	28	1
1:A:65:GLU:OE1	1:A:70:LYS:CA	0.44	2.66	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:ASP:HA	1:B:87:ARG:HD2	0.44	1.89	25	1
1:A:5:LEU:N	1:A:5:LEU:HD23	0.44	2.28	3	1
1:B:90:LEU:HB3	1:B:95:ALA:HB3	0.44	1.89	27	1
1:A:19:LEU:O	1:A:20:LYS:HG2	0.44	2.13	11	3
1:B:34:GLU:CA	1:B:80:THR:HG23	0.44	2.43	16	1
1:A:7:GLN:O	1:A:9:PRO:HD3	0.44	2.12	25	2
1:A:83:ASN:O	1:A:84:ILE:HG12	0.44	2.13	14	1
1:B:21:GLU:O	1:B:83:ASN:CG	0.44	2.56	1	2
1:A:13:ILE:HG22	1:A:66:ILE:HG12	0.44	1.88	6	1
1:B:60:ASP:OD1	1:B:74:THR:OG1	0.44	2.34	21	2
1:B:88:ASN:CG	1:B:89:LEU:N	0.44	2.71	19	2
1:A:5:LEU:C	1:A:7:GLN:N	0.44	2.71	18	5
1:A:93:ILE:HD12	1:B:99:PHE:CD1	0.44	2.48	22	1
1:A:29:ASP:OD2	1:B:8:ARG:NH2	0.44	2.51	5	1
1:A:38:LEU:HD23	1:A:59:TYR:CE1	0.44	2.48	5	1
1:B:16:GLY:O	1:B:17:GLY:C	0.44	2.56	26	1
1:A:45:LYS:HE2	1:A:76:LEU:HD21	0.44	1.89	20	1
1:A:87:ARG:HD3	1:B:9:PRO:HD3	0.44	1.89	21	1
1:B:42:TRP:CE3	1:B:57:ARG:CB	0.44	3.01	18	1
1:A:5:LEU:HA	1:B:87:ARG:CZ	0.44	2.43	3	1
1:A:45:LYS:HG2	1:A:56:VAL:HG23	0.44	1.90	27	1
1:A:34:GLU:OE2	1:A:81:PRO:C	0.43	2.56	23	1
1:A:31:THR:C	1:A:76:LEU:HD12	0.43	2.32	16	1
1:A:1:PRO:HD2	1:B:99:PHE:OXT	0.43	2.13	10	2
1:B:16:GLY:O	1:B:18:GLN:HG2	0.43	2.13	11	1
1:A:5:LEU:O	1:A:7:GLN:HB2	0.43	2.12	13	5
1:A:38:LEU:CD1	1:A:39:PRO:CD	0.43	2.96	1	1
1:A:65:GLU:HG2	1:A:69:HIS:O	0.43	2.13	19	1
1:B:36:MET:CE	1:B:38:LEU:HG	0.43	2.43	24	1
1:A:57:ARG:HG2	1:A:77:VAL:O	0.43	2.13	10	1
1:A:66:ILE:O	1:A:69:HIS:N	0.43	2.51	17	1
1:A:27:GLY:HA2	1:B:24:LEU:O	0.43	2.13	17	1
1:A:48:GLY:HA3	1:A:53:PHE:CE1	0.43	2.48	26	1
1:B:14:LYS:HE3	1:B:19:LEU:CG	0.43	2.43	8	1
1:B:20:LYS:HB2	1:B:83:ASN:ND2	0.43	2.27	2	4
1:A:66:ILE:O	1:A:67:CYS:CB	0.43	2.66	14	1
1:B:25:ASP:O	1:B:86:GLY:HA2	0.43	2.13	14	2
1:B:46:MET:HA	1:B:54:ILE:O	0.43	2.13	9	2
1:A:15:ILE:CG1	1:A:64:ILE:HG13	0.43	2.43	22	1
1:B:46:MET:CE	1:B:55:LYS:HG3	0.43	2.43	4	2
1:A:29:ASP:HA	1:A:87:ARG:CG	0.43	2.43	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:PRO:HD3	1:A:69:HIS:NE2	0.43	2.27	3	2
1:B:58:GLN:HG3	1:B:60:ASP:OD1	0.43	2.13	26	1
1:B:71:ALA:CB	1:B:89:LEU:CD1	0.43	2.96	20	1
1:A:57:ARG:HB2	1:A:59:TYR:CE2	0.43	2.48	1	2
1:A:99:PHE:OXT	1:B:1:PRO:HD2	0.43	2.13	8	2
1:A:47:ILE:HG12	1:A:54:ILE:HG13	0.43	1.90	7	1
1:B:26:THR:HG22	1:B:87:ARG:NH1	0.43	2.27	11	1
1:A:6:TRP:CE3	1:B:91:THR:HB	0.43	2.47	13	1
1:B:45:LYS:HG2	1:B:56:VAL:HG23	0.43	1.90	28	2
1:B:34:GLU:OE2	1:B:80:THR:O	0.43	2.36	6	1
1:A:33:LEU:HG	1:A:83:ASN:OD1	0.43	2.13	26	3
1:B:62:ILE:HD13	1:B:75:VAL:CG2	0.43	2.32	17	2
1:A:6:TRP:CZ2	1:B:91:THR:HB	0.43	2.48	17	1
1:A:58:GLN:OE1	1:A:76:LEU:CG	0.43	2.67	28	1
1:B:47:ILE:HG13	1:B:54:ILE:HG12	0.43	1.90	26	3
1:B:24:LEU:HD23	1:B:85:ILE:CB	0.43	2.43	27	2
1:B:88:ASN:OD1	1:B:89:LEU:HG	0.43	2.13	16	1
1:A:33:LEU:N	1:A:76:LEU:O	0.43	2.52	2	5
1:A:40:GLY:O	1:A:41:ARG:O	0.43	2.36	13	1
1:A:87:ARG:CG	1:A:87:ARG:NH1	0.43	2.80	5	1
1:A:29:ASP:HA	1:A:87:ARG:HG2	0.43	1.89	17	1
1:A:46:MET:HA	1:A:54:ILE:O	0.43	2.13	15	3
1:A:99:PHE:HB2	1:B:93:ILE:HB	0.43	1.89	28	3
1:B:9:PRO:O	1:B:24:LEU:HB2	0.43	2.14	25	2
1:A:97:LEU:HD23	1:B:24:LEU:HD13	0.43	1.89	18	1
1:A:5:LEU:CD1	1:B:97:LEU:HD13	0.43	2.44	3	1
1:A:30:ASP:OD2	1:A:74:THR:HB	0.43	2.14	4	1
1:A:10:LEU:C	1:A:11:VAL:CG1	0.43	2.87	1	4
1:B:86:GLY:O	1:B:90:LEU:HG	0.43	2.14	4	2
1:B:58:GLN:HG3	1:B:74:THR:HG21	0.43	1.91	14	1
1:A:88:ASN:CG	1:A:89:LEU:N	0.43	2.71	22	1
1:B:15:ILE:HG22	1:B:38:LEU:HD11	0.43	1.89	22	1
1:B:46:MET:CG	1:B:55:LYS:HG2	0.43	2.43	4	1
1:A:42:TRP:CE3	1:A:42:TRP:O	0.43	2.72	23	1
1:A:54:ILE:CG2	1:B:51:GLY:CA	0.43	2.97	23	3
1:A:11:VAL:HG21	1:A:66:ILE:CG1	0.43	2.43	16	1
1:A:46:MET:SD	1:A:55:LYS:HA	0.43	2.53	13	1
1:A:72:ILE:O	1:A:92:GLN:CD	0.43	2.56	13	1
1:B:31:THR:HG22	1:B:33:LEU:HD12	0.43	1.90	15	3
1:B:34:GLU:CA	1:B:80:THR:CG2	0.43	2.96	26	3
1:B:50:ILE:CD1	2:B:100:DMP:H62	0.43	2.44	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:57:ARG:HG2	1:B:77:VAL:HB	0.43	1.89	19	1
1:B:15:ILE:HD12	1:B:75:VAL:HG21	0.43	1.91	24	1
1:B:21:GLU:CD	1:B:21:GLU:N	0.43	2.71	24	1
1:A:38:LEU:HD12	1:A:39:PRO:HD3	0.43	1.89	26	2
1:A:42:TRP:CG	1:A:59:TYR:CE1	0.43	3.06	17	1
1:B:82:VAL:HG12	1:B:84:ILE:CG1	0.43	2.43	28	1
1:B:60:ASP:C	1:B:61:GLN:HG3	0.43	2.34	26	1
1:A:45:LYS:NZ	1:A:45:LYS:N	0.43	2.67	15	1
1:B:63:LEU:HD23	1:B:64:ILE:N	0.43	2.28	21	1
1:B:34:GLU:HB3	1:B:80:THR:O	0.43	2.14	21	1
1:B:60:ASP:O	1:B:61:GLN:HG3	0.43	2.13	25	1
1:A:87:ARG:NH2	1:A:87:ARG:HB2	0.43	2.29	4	1
1:B:26:THR:HA	1:B:90:LEU:HD12	0.43	1.90	23	2
1:A:83:ASN:C	1:A:84:ILE:HG12	0.43	2.33	16	1
1:B:14:LYS:O	1:B:64:ILE:HA	0.43	2.13	16	1
1:A:87:ARG:CZ	1:A:87:ARG:CB	0.43	2.97	24	1
1:A:45:LYS:O	1:A:56:VAL:HG23	0.43	2.13	20	1
1:A:14:LYS:CD	1:A:19:LEU:CD2	0.43	2.93	25	2
1:B:57:ARG:HD3	1:B:77:VAL:O	0.43	2.14	18	1
1:A:25:ASP:OD2	1:A:84:ILE:HG23	0.43	2.14	7	1
1:A:47:ILE:HD11	1:A:54:ILE:CG1	0.43	2.44	18	3
1:A:11:VAL:HG21	1:A:66:ILE:HG13	0.43	1.89	1	1
1:B:88:ASN:CG	1:B:89:LEU:HD23	0.43	2.33	1	1
1:A:99:PHE:CD2	1:B:1:PRO:HG2	0.43	2.49	6	1
1:A:35:GLU:HA	1:A:77:VAL:HG13	0.43	1.91	19	2
1:B:93:ILE:CD1	1:B:95:ALA:HB2	0.43	2.43	24	1
1:A:46:MET:CA	1:A:54:ILE:O	0.43	2.67	9	1
1:A:67:CYS:O	1:A:68:GLY:C	0.43	2.57	9	1
1:A:14:LYS:CG	1:A:18:GLN:O	0.43	2.66	10	1
1:B:13:ILE:HB	1:B:64:ILE:HG13	0.43	1.89	26	2
1:B:56:VAL:CA	1:B:77:VAL:O	0.43	2.67	20	1
1:B:87:ARG:NH2	1:B:91:THR:CG2	0.43	2.82	15	1
1:B:29:ASP:O	1:B:87:ARG:HD2	0.43	2.14	25	1
1:B:10:LEU:C	1:B:11:VAL:CG1	0.43	2.86	27	1
1:B:72:ILE:O	1:B:92:GLN:CD	0.43	2.57	23	2
1:A:26:THR:OG1	1:B:26:THR:CB	0.43	2.67	16	1
1:A:6:TRP:O	1:A:7:GLN:HG2	0.43	2.14	16	2
1:A:47:ILE:O	1:A:47:ILE:HG13	0.43	2.14	8	1
1:B:86:GLY:O	1:B:88:ASN:OD1	0.43	2.37	7	1
1:B:66:ILE:CD1	1:B:89:LEU:HD12	0.43	2.44	9	1
1:A:96:THR:CG2	1:B:4:THR:CG2	0.43	2.94	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:ILE:HG13	1:B:54:ILE:HG13	0.43	1.90	2	1
1:B:71:ALA:HB1	1:B:89:LEU:HD13	0.43	1.90	20	1
1:A:40:GLY:O	1:A:41:ARG:HG2	0.43	2.14	18	1
1:B:13:ILE:CG2	1:B:22:ALA:HB3	0.43	2.44	4	1
1:A:20:LYS:CB	1:A:83:ASN:ND2	0.43	2.82	12	3
1:A:85:ILE:HG23	1:A:89:LEU:HB2	0.43	1.91	14	2
1:B:38:LEU:HD11	1:B:77:VAL:HG21	0.43	1.91	12	1
1:B:28:ALA:HB1	2:B:100:DMP:C75	0.43	2.44	8	1
1:A:45:LYS:HG3	1:A:56:VAL:HG22	0.43	1.91	8	1
1:A:46:MET:HG2	1:A:54:ILE:O	0.43	2.14	11	2
1:A:93:ILE:CD1	1:B:99:PHE:HB2	0.43	2.35	11	1
1:B:11:VAL:CG2	1:B:11:VAL:O	0.43	2.67	11	3
1:A:6:TRP:CD1	1:A:6:TRP:N	0.43	2.85	1	2
1:A:18:GLN:NE2	1:A:37:SER:HB3	0.43	2.29	14	2
1:A:22:ALA:HA	1:A:83:ASN:CB	0.43	2.44	19	2
1:A:5:LEU:O	1:B:87:ARG:HD2	0.43	2.14	24	1
1:A:15:ILE:CD1	1:A:64:ILE:HB	0.43	2.44	22	1
1:A:85:ILE:HG22	1:A:90:LEU:HD23	0.43	1.91	28	1
1:B:46:MET:HB3	1:B:54:ILE:O	0.43	2.14	2	1
1:A:99:PHE:O	1:B:1:PRO:HD2	0.43	2.14	26	1
1:A:58:GLN:HA	1:A:75:VAL:O	0.43	2.14	20	1
1:A:57:ARG:N	1:A:77:VAL:O	0.43	2.51	27	1
1:A:50:ILE:CD1	2:B:100:DMP:H32	0.43	2.43	27	1
1:A:99:PHE:CG	1:B:93:ILE:HD13	0.42	2.49	16	1
1:A:60:ASP:C	1:A:61:GLN:CG	0.42	2.87	16	2
1:B:54:ILE:CD1	1:B:80:THR:HB	0.42	2.43	13	1
1:A:99:PHE:O	1:B:93:ILE:O	0.42	2.37	5	2
1:B:66:ILE:O	1:B:67:CYS:C	0.42	2.56	5	2
1:A:38:LEU:CD1	1:A:39:PRO:HD3	0.42	2.44	1	1
1:A:40:GLY:O	1:A:41:ARG:CG	0.42	2.67	18	2
1:A:18:GLN:OE1	1:A:37:SER:O	0.42	2.36	6	1
1:A:95:ALA:O	1:B:5:LEU:CD1	0.42	2.66	6	1
1:A:38:LEU:HA	1:A:38:LEU:HD12	0.42	1.69	6	1
1:B:15:ILE:HG22	1:B:15:ILE:O	0.42	2.13	24	1
1:A:45:LYS:HB2	1:A:56:VAL:O	0.42	2.14	17	1
1:B:90:LEU:O	1:B:95:ALA:N	0.42	2.51	17	1
1:B:14:LYS:CE	1:B:19:LEU:HD11	0.42	2.44	17	1
1:A:83:ASN:C	1:A:84:ILE:HG13	0.42	2.34	20	1
1:B:5:LEU:CD2	1:B:9:PRO:HA	0.42	2.43	21	1
1:A:29:ASP:OD2	1:A:87:ARG:NH1	0.42	2.51	27	1
1:B:38:LEU:HB3	1:B:39:PRO:CD	0.42	2.43	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:14:LYS:HG3	1:B:19:LEU:CD1	0.42	2.43	12	1
1:A:5:LEU:O	1:A:7:GLN:HG3	0.42	2.13	7	1
1:A:25:ASP:OD1	2:B:100:DMP:C4	0.42	2.67	11	1
1:B:32:VAL:HG12	1:B:84:ILE:CB	0.42	2.43	14	1
1:A:95:ALA:O	1:B:5:LEU:HD12	0.42	2.14	6	1
1:A:31:THR:HG23	1:A:85:ILE:HA	0.42	1.91	22	1
1:A:46:MET:SD	1:A:53:PHE:HB3	0.42	2.54	18	2
1:B:67:CYS:O	1:B:69:HIS:NE2	0.42	2.52	17	1
1:B:54:ILE:O	1:B:54:ILE:HG13	0.42	2.14	15	1
1:A:5:LEU:HB3	1:B:87:ARG:CG	0.42	2.44	3	1
1:A:15:ILE:CG1	1:A:64:ILE:CB	0.42	2.97	27	1
1:B:11:VAL:O	1:B:11:VAL:CG2	0.42	2.68	28	2
1:A:26:THR:CG2	1:A:87:ARG:NH2	0.42	2.83	23	1
1:A:14:LYS:O	1:A:64:ILE:HA	0.42	2.14	16	1
1:A:5:LEU:O	1:B:87:ARG:CD	0.42	2.66	11	1
1:A:46:MET:SD	1:A:55:LYS:HG3	0.42	2.54	13	1
1:B:14:LYS:HG3	1:B:19:LEU:CG	0.42	2.44	10	1
1:A:11:VAL:O	1:A:22:ALA:N	0.42	2.52	17	1
1:A:63:LEU:HD23	1:A:72:ILE:HG12	0.42	1.91	28	1
1:B:25:ASP:OD1	1:B:25:ASP:C	0.42	2.57	26	1
1:A:9:PRO:HG2	1:A:24:LEU:HB2	0.42	1.91	4	1
1:B:34:GLU:CG	1:B:35:GLU:N	0.42	2.82	23	1
1:A:54:ILE:HG23	1:B:51:GLY:N	0.42	2.29	23	1
1:A:87:ARG:O	1:A:89:LEU:N	0.42	2.53	21	2
1:A:47:ILE:O	1:A:53:PHE:CB	0.42	2.68	8	1
1:A:6:TRP:N	1:A:6:TRP:CD1	0.42	2.87	19	1
1:B:68:GLY:C	1:B:69:HIS:CD2	0.42	2.93	22	1
1:B:38:LEU:HD13	1:B:39:PRO:HD3	0.42	1.92	17	2
1:B:14:LYS:HG3	1:B:19:LEU:HG	0.42	1.91	10	1
1:B:32:VAL:HG21	1:B:47:ILE:HD13	0.42	1.90	15	2
1:A:46:MET:HG3	1:A:55:LYS:HG2	0.42	1.91	10	1
1:B:15:ILE:CG2	1:B:38:LEU:HD11	0.42	2.45	20	1
1:A:87:ARG:HG2	1:B:7:GLN:O	0.42	2.14	15	1
1:B:87:ARG:HA	1:B:87:ARG:NE	0.42	2.29	27	1
1:A:66:ILE:O	1:A:69:HIS:HB2	0.42	2.14	16	1
1:A:2:GLN:NE2	1:A:4:THR:CG2	0.42	2.83	16	1
1:A:59:TYR:C	1:A:62:ILE:CD1	0.42	2.88	9	2
1:A:30:ASP:OD1	1:A:88:ASN:HB3	0.42	2.15	14	3
1:A:36:MET:HG3	1:A:38:LEU:CD2	0.42	2.44	1	1
1:A:30:ASP:O	1:A:86:GLY:CA	0.42	2.68	5	1
1:B:19:LEU:O	1:B:20:LYS:HD3	0.42	2.15	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ASP:OD2	1:A:84:ILE:CG2	0.42	2.68	7	1
1:A:63:LEU:HD11	1:A:70:LYS:CA	0.42	2.44	7	1
1:B:5:LEU:O	1:B:7:GLN:HG3	0.42	2.14	7	1
1:A:93:ILE:HD13	1:B:99:PHE:CG	0.42	2.50	24	1
1:A:34:GLU:OE1	1:A:35:GLU:N	0.42	2.53	22	1
1:B:1:PRO:HD3	1:B:69:HIS:NE2	0.42	2.29	28	2
1:A:65:GLU:OE1	1:A:69:HIS:C	0.42	2.58	18	1
1:A:97:LEU:CD2	1:B:24:LEU:HD13	0.42	2.45	18	1
1:A:1:PRO:HG2	1:B:99:PHE:CD2	0.42	2.50	25	1
1:A:25:ASP:OD1	1:A:25:ASP:C	0.42	2.57	3	1
1:B:56:VAL:CG2	1:B:76:LEU:HB3	0.42	2.45	16	1
1:B:5:LEU:O	1:B:7:GLN:HB2	0.42	2.14	25	3
1:A:14:LYS:HG3	1:A:19:LEU:HD12	0.42	1.91	9	2
1:A:57:ARG:O	1:A:76:LEU:HD23	0.42	2.15	13	1
1:A:66:ILE:O	1:A:67:CYS:HB2	0.42	2.14	6	5
1:A:4:THR:O	1:A:5:LEU:HG	0.42	2.15	14	1
1:A:13:ILE:CD1	1:A:15:ILE:HG13	0.42	2.44	1	1
1:A:46:MET:CE	1:A:55:LYS:HG3	0.42	2.45	22	1
1:A:45:LYS:O	1:A:45:LYS:HG3	0.42	2.13	9	1
1:A:25:ASP:OD2	2:B:100:DMP:O4	0.42	2.37	10	1
1:A:38:LEU:HA	1:A:38:LEU:HD23	0.42	1.73	2	1
1:B:45:LYS:CE	1:B:76:LEU:CD2	0.42	2.88	26	1
1:B:57:ARG:HB2	1:B:59:TYR:CE2	0.42	2.50	20	1
1:B:32:VAL:CG1	1:B:33:LEU:N	0.42	2.81	25	2
1:B:90:LEU:O	1:B:93:ILE:HG13	0.42	2.15	3	1
1:B:54:ILE:CD1	1:B:79:PRO:HD2	0.42	2.45	4	1
1:A:34:GLU:OE2	1:A:34:GLU:O	0.42	2.38	12	1
1:A:46:MET:CE	1:A:55:LYS:HE3	0.42	2.45	12	1
1:A:15:ILE:HG13	1:A:64:ILE:HG13	0.42	1.90	17	2
1:B:3:VAL:CG1	1:B:5:LEU:HB2	0.42	2.44	23	1
1:A:90:LEU:O	1:A:95:ALA:CB	0.42	2.61	13	1
1:A:96:THR:HG22	1:B:4:THR:HG21	0.42	1.88	13	1
1:A:16:GLY:O	1:A:18:GLN:OE1	0.42	2.38	14	1
1:B:57:ARG:HG3	1:B:77:VAL:O	0.42	2.14	21	3
1:A:11:VAL:CG2	1:A:66:ILE:HG23	0.42	2.45	6	1
1:A:95:ALA:HA	1:B:99:PHE:HB3	0.42	1.92	6	1
1:B:61:GLN:NE2	1:B:61:GLN:HA	0.42	2.29	24	1
1:B:3:VAL:HG12	1:B:3:VAL:O	0.42	2.15	9	1
1:A:99:PHE:O	1:B:1:PRO:CD	0.42	2.67	17	1
1:A:14:LYS:CB	1:A:65:GLU:HB3	0.42	2.44	26	1
1:B:23:LEU:N	1:B:83:ASN:O	0.42	2.53	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:31:THR:HG23	1:B:85:ILE:CD1	0.42	2.44	25	1
1:A:31:THR:O	1:A:75:VAL:HA	0.42	2.15	27	1
1:B:31:THR:CG2	1:B:84:ILE:O	0.42	2.66	12	1
1:B:38:LEU:HD23	1:B:39:PRO:HD3	0.42	1.92	19	1
1:B:68:GLY:O	1:B:69:HIS:CG	0.42	2.72	22	1
1:A:87:ARG:HG2	1:A:87:ARG:NH1	0.42	2.30	5	1
1:B:26:THR:CG2	1:B:87:ARG:NH2	0.42	2.82	5	1
1:B:33:LEU:O	1:B:77:VAL:HA	0.42	2.15	26	1
1:A:54:ILE:CG2	1:B:50:ILE:HG23	0.42	2.44	18	1
1:A:34:GLU:O	1:A:34:GLU:OE1	0.42	2.37	25	1
1:A:31:THR:HG22	1:A:33:LEU:HD13	0.42	1.90	3	1
1:A:51:GLY:HA2	1:B:54:ILE:HG22	0.42	1.92	12	1
1:B:46:MET:HG2	1:B:55:LYS:HG2	0.42	1.92	16	1
1:A:31:THR:OG1	1:A:75:VAL:HA	0.42	2.15	13	1
1:A:10:LEU:HD23	1:A:22:ALA:H	0.42	1.74	13	1
1:B:30:ASP:OD2	1:B:74:THR:HB	0.42	2.14	14	1
1:A:34:GLU:HB3	1:A:80:THR:O	0.42	2.14	20	3
1:B:36:MET:CG	1:B:37:SER:N	0.42	2.82	15	2
1:A:95:ALA:O	1:B:5:LEU:CG	0.42	2.68	6	1
1:A:65:GLU:CG	1:A:69:HIS:O	0.42	2.68	19	1
1:B:4:THR:C	1:B:6:TRP:N	0.42	2.73	24	3
1:A:8:ARG:HB3	1:A:23:LEU:CD1	0.42	2.45	20	2
1:B:46:MET:CA	1:B:54:ILE:O	0.42	2.67	9	1
1:B:38:LEU:HA	1:B:38:LEU:HD12	0.42	1.74	10	1
1:A:31:THR:CG2	1:A:31:THR:O	0.42	2.67	17	1
1:A:3:VAL:CG1	1:A:9:PRO:CB	0.42	2.98	20	1
1:A:87:ARG:CD	1:B:9:PRO:HD3	0.42	2.45	21	1
1:A:19:LEU:O	1:A:20:LYS:HG3	0.42	2.15	18	1
1:A:93:ILE:O	1:B:99:PHE:C	0.42	2.58	25	1
1:A:15:ILE:CD1	1:A:33:LEU:HD22	0.42	2.45	3	1
1:B:68:GLY:O	1:B:69:HIS:CD2	0.42	2.73	4	1
1:A:62:ILE:O	1:A:72:ILE:HA	0.41	2.15	13	6
1:B:15:ILE:HG12	1:B:75:VAL:HG21	0.41	1.92	13	1
1:A:99:PHE:HA	1:B:94:GLY:O	0.41	2.15	25	6
1:A:7:GLN:HA	1:B:87:ARG:NH2	0.41	2.30	6	1
1:B:45:LYS:O	1:B:46:MET:HG2	0.41	2.14	24	1
1:A:28:ALA:O	1:A:86:GLY:HA3	0.41	2.15	5	1
1:B:85:ILE:CG2	1:B:90:LEU:CD2	0.41	2.98	10	1
1:A:69:HIS:CG	1:A:93:ILE:HG22	0.41	2.50	21	1
1:A:83:ASN:O	1:A:85:ILE:HD13	0.41	2.15	21	1
1:A:7:GLN:O	1:B:87:ARG:CB	0.41	2.68	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:VAL:CG1	1:A:33:LEU:N	0.41	2.81	27	1
1:B:30:ASP:O	1:B:86:GLY:CA	0.41	2.68	16	1
1:A:58:GLN:O	1:A:58:GLN:CG	0.41	2.66	7	1
1:A:5:LEU:O	1:B:87:ARG:HD3	0.41	2.15	11	1
1:A:25:ASP:C	1:A:25:ASP:OD1	0.41	2.58	13	1
1:A:26:THR:HG23	1:A:90:LEU:CD2	0.41	2.45	6	1
1:B:64:ILE:HG12	1:B:66:ILE:CD1	0.41	2.45	5	2
1:B:7:GLN:OE1	1:B:7:GLN:HA	0.41	2.15	19	1
1:A:30:ASP:HB3	1:A:88:ASN:OD1	0.41	2.15	5	1
1:A:29:ASP:O	1:A:30:ASP:OD1	0.41	2.37	17	1
1:B:36:MET:H	1:B:77:VAL:HG11	0.41	1.74	26	1
1:A:15:ILE:HG12	1:A:64:ILE:HB	0.41	1.92	15	1
1:A:38:LEU:HG	1:A:59:TYR:CD1	0.41	2.50	18	1
1:B:46:MET:HE2	1:B:55:LYS:HG3	0.41	1.91	4	1
1:A:45:LYS:O	1:A:45:LYS:HD3	0.41	2.16	11	1
1:A:11:VAL:HG23	1:A:12:THR:N	0.41	2.29	13	1
1:A:15:ILE:CD1	1:A:36:MET:CE	0.41	2.98	24	1
1:A:39:PRO:O	1:A:41:ARG:HG2	0.41	2.15	5	1
1:A:60:ASP:N	1:A:60:ASP:OD1	0.41	2.53	10	1
1:A:63:LEU:CD2	1:A:72:ILE:HG12	0.41	2.44	10	1
1:B:66:ILE:O	1:B:69:HIS:CG	0.41	2.73	17	1
1:A:19:LEU:C	1:A:20:LYS:HG2	0.41	2.36	2	1
1:B:15:ILE:HD11	1:B:64:ILE:HB	0.41	1.91	2	1
1:B:15:ILE:O	1:B:16:GLY:C	0.41	2.58	26	1
1:A:9:PRO:O	1:A:24:LEU:HD12	0.41	2.14	4	1
1:A:6:TRP:CH2	1:B:91:THR:HB	0.41	2.50	4	1
1:A:8:ARG:HG2	1:B:29:ASP:OD2	0.41	2.15	27	1
1:A:10:LEU:CG	1:A:22:ALA:O	0.41	2.68	16	2
1:B:15:ILE:HD11	1:B:64:ILE:CD1	0.41	2.42	7	1
1:A:48:GLY:HA3	1:A:53:PHE:CZ	0.41	2.50	11	2
1:A:13:ILE:HB	1:A:64:ILE:HG13	0.41	1.91	11	3
1:A:31:THR:CG2	1:A:85:ILE:HA	0.41	2.45	13	1
1:B:38:LEU:HA	1:B:38:LEU:HD23	0.41	1.73	14	1
1:B:30:ASP:OD1	1:B:88:ASN:HB3	0.41	2.15	3	2
1:A:88:ASN:CG	1:A:89:LEU:HD23	0.41	2.33	24	1
1:A:31:THR:OG1	1:A:88:ASN:OD1	0.41	2.38	22	1
1:A:32:VAL:HG12	1:A:32:VAL:O	0.41	2.14	22	1
1:B:1:PRO:HG3	1:B:67:CYS:HB3	0.41	1.91	15	1
1:A:13:ILE:HG22	1:A:66:ILE:HD13	0.41	1.91	21	1
1:B:71:ALA:HB2	1:B:93:ILE:HG22	0.41	1.92	18	1
1:A:97:LEU:CD1	1:B:97:LEU:HD13	0.41	2.34	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:87:ARG:NH1	1:B:90:LEU:HB3	0.41	2.30	27	1
1:A:14:LYS:HB2	1:A:65:GLU:HB3	0.41	1.91	27	1
1:B:64:ILE:HD11	1:B:66:ILE:HD11	0.41	1.92	19	2
1:B:85:ILE:HG23	1:B:89:LEU:HB3	0.41	1.92	9	1
1:A:11:VAL:O	1:A:22:ALA:CB	0.41	2.68	17	1
1:A:47:ILE:HG13	1:A:54:ILE:HG12	0.41	1.92	28	1
1:B:58:GLN:HE22	1:B:74:THR:HG22	0.41	1.75	26	1
1:A:2:GLN:OE1	1:A:4:THR:CG2	0.41	2.69	26	1
1:B:76:LEU:N	1:B:76:LEU:CD1	0.41	2.80	15	1
1:B:42:TRP:CD2	1:B:57:ARG:HB3	0.41	2.50	18	1
1:B:67:CYS:HB2	1:B:69:HIS:CD2	0.41	2.51	25	1
1:A:67:CYS:O	1:A:69:HIS:CG	0.41	2.72	3	1
1:A:34:GLU:CD	1:A:80:THR:O	0.41	2.58	23	1
1:A:32:VAL:O	1:A:84:ILE:N	0.41	2.53	16	1
1:A:87:ARG:C	1:A:89:LEU:N	0.41	2.73	16	1
1:B:50:ILE:HD13	2:B:100:DMP:C26	0.41	2.44	1	1
1:A:41:ARG:CD	1:A:41:ARG:N	0.41	2.84	10	1
1:A:65:GLU:HG2	1:A:66:ILE:N	0.41	2.31	10	1
1:B:15:ILE:CD1	1:B:64:ILE:HB	0.41	2.46	2	1
1:A:7:GLN:O	1:B:87:ARG:HD3	0.41	2.15	3	1
1:A:69:HIS:O	1:A:71:ALA:N	0.41	2.53	23	1
1:A:49:GLY:HA3	2:B:100:DMP:H201	0.41	1.91	13	1
1:B:46:MET:HG2	1:B:55:LYS:HG3	0.41	1.92	22	2
1:A:11:VAL:HB	1:A:67:CYS:SG	0.41	2.56	17	1
1:A:34:GLU:HG2	1:A:35:GLU:N	0.41	2.31	2	1
1:A:2:GLN:OE1	1:A:4:THR:HG23	0.41	2.16	26	1
1:A:93:ILE:HB	1:B:99:PHE:HB2	0.41	1.92	18	1
1:A:58:GLN:OE1	1:A:60:ASP:OD1	0.41	2.37	4	1
1:B:46:MET:HE3	1:B:55:LYS:CG	0.41	2.46	4	1
1:B:66:ILE:O	1:B:69:HIS:HB2	0.41	2.16	23	2
1:A:31:THR:CG2	1:A:75:VAL:HG13	0.41	2.46	16	1
1:A:99:PHE:CD1	1:B:95:ALA:HA	0.41	2.51	16	1
1:B:47:ILE:HG13	1:B:47:ILE:O	0.41	2.14	13	1
1:A:8:ARG:HG2	1:B:29:ASP:OD1	0.41	2.16	13	1
1:A:90:LEU:HD12	1:A:90:LEU:N	0.41	2.31	6	1
1:A:34:GLU:CA	1:A:80:THR:HG23	0.41	2.46	19	1
1:B:15:ILE:O	1:B:18:GLN:HB2	0.41	2.16	26	1
1:A:98:ASN:OD1	1:B:98:ASN:OD1	0.41	2.38	21	1
1:A:13:ILE:HD12	1:A:15:ILE:CD1	0.41	2.45	23	1
1:B:85:ILE:HG23	1:B:89:LEU:HD12	0.41	1.92	16	1
1:B:30:ASP:O	1:B:86:GLY:N	0.41	2.54	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:33:LEU:HG	1:B:83:ASN:HA	0.41	1.93	11	1
1:A:58:GLN:CG	1:A:74:THR:HG22	0.41	2.46	13	1
1:A:5:LEU:CD1	1:A:7:GLN:HB2	0.41	2.44	14	1
1:A:92:GLN:OE1	1:A:92:GLN:HA	0.41	2.15	1	1
1:B:3:VAL:O	1:B:3:VAL:HG12	0.41	2.16	6	1
1:A:97:LEU:HA	1:B:96:THR:O	0.41	2.16	6	1
1:A:6:TRP:CE3	1:B:91:THR:CG2	0.41	3.03	19	1
1:A:58:GLN:C	1:A:58:GLN:CD	0.41	2.80	22	1
1:A:87:ARG:NH1	1:A:90:LEU:HB2	0.41	2.30	22	1
1:B:15:ILE:CG2	1:B:36:MET:HE3	0.41	2.46	5	1
1:B:4:THR:HG1	1:B:6:TRP:HD1	0.41	1.53	5	1
1:B:18:GLN:O	1:B:19:LEU:HG	0.41	2.16	28	1
1:B:38:LEU:HD23	1:B:59:TYR:CE2	0.41	2.51	28	1
1:A:62:ILE:N	1:A:72:ILE:HG23	0.41	2.31	20	1
1:A:59:TYR:CB	1:A:62:ILE:HG13	0.41	2.46	20	1
1:A:45:LYS:HE3	1:A:58:GLN:CB	0.41	2.46	15	1
1:B:33:LEU:HB2	1:B:75:VAL:CG1	0.41	2.43	21	1
1:A:87:ARG:NH2	1:B:9:PRO:HG3	0.41	2.31	3	1
1:A:9:PRO:HG2	1:A:24:LEU:CB	0.41	2.45	4	1
1:B:38:LEU:HD12	1:B:59:TYR:CD1	0.41	2.50	27	1
1:A:36:MET:SD	1:A:37:SER:C	0.41	2.99	27	1
1:A:9:PRO:O	1:A:24:LEU:HG	0.41	2.15	12	1
1:A:46:MET:CG	1:A:55:LYS:CG	0.41	2.99	21	1
1:B:26:THR:HG23	1:B:87:ARG:CD	0.41	2.46	27	1
1:B:12:THR:HG21	1:B:19:LEU:CD2	0.40	2.46	12	1
1:A:23:LEU:O	1:A:23:LEU:HG	0.40	2.16	8	2
1:B:57:ARG:HG2	1:B:57:ARG:NH1	0.40	2.30	11	1
1:A:46:MET:SD	1:A:55:LYS:N	0.40	2.95	13	1
1:B:81:PRO:C	1:B:82:VAL:HG23	0.40	2.36	22	1
1:B:10:LEU:CD2	1:B:21:GLU:C	0.40	2.89	20	1
1:A:36:MET:SD	1:A:38:LEU:CD2	0.40	3.09	18	1
1:A:9:PRO:CG	1:A:24:LEU:HB2	0.40	2.45	27	1
1:A:87:ARG:CA	1:A:90:LEU:HD23	0.40	2.44	7	1
1:A:4:THR:C	1:A:5:LEU:HG	0.40	2.36	19	2
1:A:61:GLN:CA	1:A:61:GLN:NE2	0.40	2.83	14	1
1:A:45:LYS:HD3	1:A:76:LEU:CD2	0.40	2.46	14	1
1:A:15:ILE:CG2	1:A:36:MET:HE3	0.40	2.46	6	1
1:B:5:LEU:O	1:B:5:LEU:HG	0.40	2.15	22	1
1:A:31:THR:CG2	1:A:33:LEU:HD11	0.40	2.46	5	1
1:A:87:ARG:NH1	1:B:7:GLN:HA	0.40	2.31	10	1
1:A:58:GLN:OE1	1:A:76:LEU:HG	0.40	2.16	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:N	1:A:62:ILE:CD1	0.40	2.81	2	1
1:A:8:ARG:NH2	1:B:26:THR:O	0.40	2.54	26	1
1:A:87:ARG:HD3	1:B:7:GLN:O	0.40	2.16	15	1
1:B:87:ARG:C	1:B:89:LEU:N	0.40	2.75	25	2
1:B:13:ILE:HG13	1:B:13:ILE:O	0.40	2.16	27	1
1:A:10:LEU:CD2	1:A:22:ALA:O	0.40	2.69	16	1
1:A:13:ILE:O	1:A:13:ILE:HG13	0.40	2.16	5	3
1:A:41:ARG:NH1	1:A:41:ARG:HG3	0.40	2.30	11	1
1:A:59:TYR:CE2	1:A:77:VAL:HG21	0.40	2.51	13	1
1:B:38:LEU:CD1	1:B:59:TYR:CD1	0.40	3.04	14	1
1:B:65:GLU:OE2	1:B:68:GLY:HA2	0.40	2.16	17	2
1:A:63:LEU:HA	1:A:72:ILE:HG13	0.40	1.92	22	1
1:A:4:THR:C	1:A:6:TRP:N	0.40	2.74	26	2
1:B:34:GLU:CD	1:B:81:PRO:C	0.40	2.80	2	1
1:B:88:ASN:O	1:B:92:GLN:HG3	0.40	2.16	25	1
1:B:97:LEU:O	1:B:99:PHE:CD1	0.40	2.73	3	1
1:A:5:LEU:O	1:A:5:LEU:HG	0.40	2.15	4	1
1:A:59:TYR:HB2	1:A:75:VAL:O	0.40	2.17	27	1
1:A:10:LEU:HD23	1:A:22:ALA:O	0.40	2.16	16	1
1:A:42:TRP:O	1:A:43:LYS:HG2	0.40	2.17	16	1
1:A:52:GLY:O	1:B:51:GLY:HA3	0.40	2.17	5	1
1:B:19:LEU:C	1:B:20:LYS:CG	0.40	2.88	9	1
1:A:98:ASN:O	1:B:96:THR:N	0.40	2.55	10	1
1:A:3:VAL:HG11	1:A:9:PRO:HB3	0.40	1.93	28	1
1:B:25:ASP:HB3	1:B:85:ILE:O	0.40	2.15	26	1
1:B:66:ILE:HG22	1:B:66:ILE:O	0.40	2.16	27	1
1:B:59:TYR:CD1	1:B:77:VAL:HG23	0.40	2.51	14	1
1:A:7:GLN:HA	1:A:7:GLN:OE1	0.40	2.15	14	1
1:B:36:MET:SD	1:B:37:SER:C	0.40	3.00	6	1
1:A:3:VAL:HG12	1:A:5:LEU:N	0.40	2.30	6	1
1:B:36:MET:CG	1:B:38:LEU:CD2	0.40	3.00	9	1
1:A:12:THR:HG21	1:A:19:LEU:CD2	0.40	2.46	9	1
1:A:58:GLN:HG2	1:A:74:THR:HG22	0.40	1.93	9	1
1:B:63:LEU:HD13	1:B:72:ILE:HG13	0.40	1.92	26	1
1:B:28:ALA:O	1:B:87:ARG:HG3	0.40	2.17	20	1
1:B:57:ARG:O	1:B:59:TYR:CD2	0.40	2.75	3	1
1:A:28:ALA:HB1	2:B:100:DMP:C25	0.40	2.47	27	1
1:B:87:ARG:NE	1:B:90:LEU:HB2	0.40	2.31	27	1
1:B:45:LYS:O	1:B:45:LYS:HG3	0.40	2.17	27	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	97/99 (98%)	77±2 (80±2%)	15±2 (15±2%)	5±1 (5±1%)	5	26
1	B	97/99 (98%)	77±3 (80±3%)	14±3 (15±3%)	5±2 (6±2%)	4	24
All	All	5432/5544 (98%)	4328 (80%)	818 (15%)	286 (5%)	4	25

All 35 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	34	GLU	22
1	B	5	LEU	21
1	B	34	GLU	20
1	A	6	TRP	20
1	B	6	TRP	19
1	A	24	LEU	18
1	B	24	LEU	17
1	A	5	LEU	15
1	A	61	GLN	15
1	B	61	GLN	14
1	B	40	GLY	13
1	A	58	GLN	10
1	B	58	GLN	9
1	A	40	GLY	8
1	B	41	ARG	7
1	B	87	ARG	6
1	B	67	CYS	6
1	A	41	ARG	6
1	A	67	CYS	4
1	B	16	GLY	4
1	B	63	LEU	4
1	A	39	PRO	4
1	A	63	LEU	3
1	B	4	THR	3
1	B	35	GLU	3
1	A	87	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	4	THR	2
1	A	7	GLN	2
1	B	39	PRO	2
1	B	7	GLN	2
1	A	70	LYS	1
1	A	69	HIS	1
1	A	36	MET	1
1	A	35	GLU	1
1	A	16	GLY	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	82/82 (100%)	59±4 (72±4%)	23±4 (28±4%)	2	21
1	B	82/82 (100%)	60±3 (73±4%)	22±3 (27±4%)	2	23
All	All	4592/4592 (100%)	3334 (73%)	1258 (27%)	2	22

All 133 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	72	ILE	28
1	B	32	VAL	28
1	A	99	PHE	28
1	B	99	PHE	28
1	B	33	LEU	27
1	A	32	VAL	27
1	B	72	ILE	26
1	A	30	ASP	24
1	A	10	LEU	23
1	A	33	LEU	22
1	B	30	ASP	21
1	A	85	ILE	21
1	B	10	LEU	20
1	A	35	GLU	20
1	B	45	LYS	19

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Mol	Chain	Res	Type	Models (Total)
1	A	5	LEU	18
1	B	70	LYS	18
1	B	4	THR	18
1	A	70	LYS	18
1	B	66	ILE	18
1	A	45	LYS	17
1	A	82	VAL	17
1	A	66	ILE	16
1	A	41	ARG	16
1	A	4	THR	15
1	A	60	ASP	15
1	B	5	LEU	15
1	A	83	ASN	15
1	B	83	ASN	15
1	B	85	ILE	15
1	A	87	ARG	14
1	A	46	MET	14
1	A	43	LYS	13
1	A	11	VAL	13
1	A	36	MET	13
1	B	53	PHE	13
1	B	11	VAL	13
1	A	20	LYS	13
1	B	36	MET	13
1	B	93	ILE	13
1	A	93	ILE	12
1	A	91	THR	12
1	B	43	LYS	12
1	A	55	LYS	12
1	B	18	GLN	11
1	B	8	ARG	11
1	B	91	THR	11
1	B	55	LYS	11
1	A	57	ARG	11
1	B	87	ARG	11
1	B	61	GLN	11
1	B	35	GLU	11
1	A	61	GLN	11
1	B	26	THR	11
1	A	14	LYS	10
1	B	7	GLN	10
1	B	21	GLU	10

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Mol	Chain	Res	Type	Models (Total)
1	B	14	LYS	10
1	A	7	GLN	10
1	B	82	VAL	10
1	A	65	GLU	10
1	B	41	ARG	9
1	B	20	LYS	9
1	B	60	ASP	9
1	B	97	LEU	9
1	B	46	MET	9
1	A	34	GLU	8
1	A	8	ARG	8
1	B	89	LEU	8
1	A	38	LEU	8
1	A	2	GLN	8
1	A	63	LEU	7
1	B	67	CYS	7
1	A	18	GLN	7
1	A	58	GLN	7
1	B	2	GLN	7
1	A	67	CYS	7
1	B	63	LEU	7
1	B	98	ASN	6
1	B	58	GLN	6
1	A	26	THR	6
1	A	29	ASP	6
1	B	38	LEU	6
1	A	89	LEU	6
1	B	57	ARG	6
1	B	80	THR	5
1	B	75	VAL	5
1	B	62	ILE	5
1	B	34	GLU	4
1	B	29	ASP	4
1	A	53	PHE	4
1	A	21	GLU	4
1	A	24	LEU	4
1	A	15	ILE	3
1	A	90	LEU	3
1	A	19	LEU	3
1	A	80	THR	3
1	A	88	ASN	3
1	B	15	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	92	GLN	3
1	A	13	ILE	3
1	B	19	LEU	3
1	A	54	ILE	3
1	B	90	LEU	3
1	B	77	VAL	3
1	A	56	VAL	2
1	A	75	VAL	2
1	B	64	ILE	2
1	A	62	ILE	2
1	B	54	ILE	2
1	B	56	VAL	2
1	B	24	LEU	2
1	B	12	THR	2
1	B	65	GLU	2
1	B	76	LEU	2
1	A	69	HIS	2
1	B	23	LEU	2
1	B	92	GLN	2
1	A	25	ASP	2
1	A	31	THR	2
1	B	84	ILE	1
1	B	47	ILE	1
1	A	98	ASN	1
1	A	23	LEU	1
1	B	25	ASP	1
1	A	74	THR	1
1	B	6	TRP	1
1	A	6	TRP	1
1	A	76	LEU	1
1	B	13	ILE	1
1	B	42	TRP	1
1	A	97	LEU	1
1	A	12	THR	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 carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	DMP	B	100	-	46,46,46	0.63±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DMP	B	100	-	56,63,63	0.96±0.02	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DMP	B	100	-	-	0±0,20,48,48	0±0,5,5,5

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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

No chemical shift data were provided