



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 22, 2021 – 08:09 AM EDT

PDB ID : 7LOI  
Title : Model of the HIV-1 gp41 membrane-proximal external region, transmembrane domain and cytoplasmic tail  
Authors : Piai, A.; Fu, Q.; Sharp, A.K.; Bighi, B.; Brown, A.M.; Chou, J.J.  
Deposited on : 2021-02-10

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

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

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.18
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

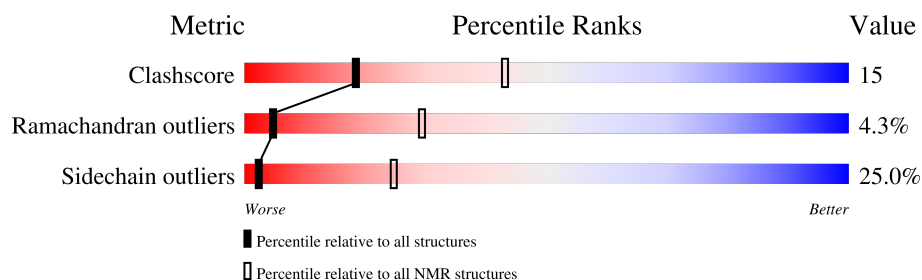
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 9%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	197	<div> <div>46%</div> <div>39%</div> <div>•</div> <div>11%</div> </div>
1	B	197	<div> <div>48%</div> <div>39%</div> <div>•</div> <div>11%</div> </div>
1	C	197	<div> <div>49%</div> <div>38%</div> <div>•</div> <div>11%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:660-A:716, A:739-A:856, B:660-B:716, B:739-B:856, C:660-C:716, C:739-C:856 (525)	0.91	4

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 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8940 atoms, of which 4563 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					Trace
1	A	175	Total	C	H	N	O	0
			2980	949	1521	267	243	
1	B	175	Total	C	H	N	O	0
			2980	949	1521	267	243	
1	C	175	Total	C	H	N	O	0
			2980	949	1521	267	243	

There are 27 discrepancies between the modelled and reference sequences:

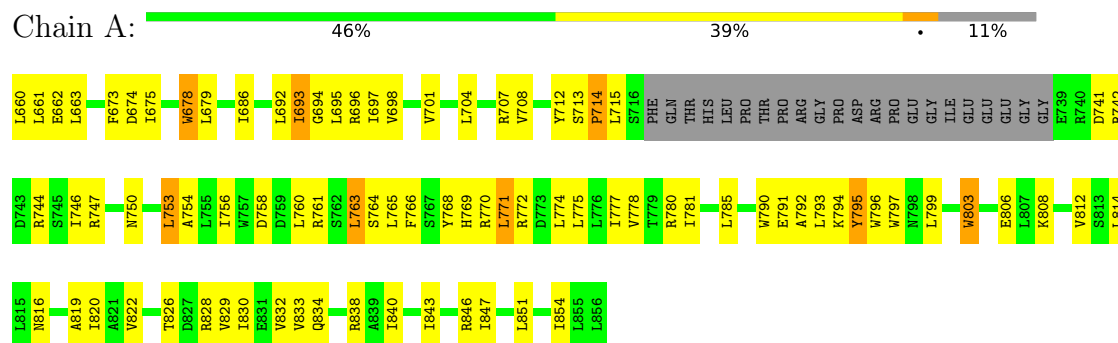
Chain	Residue	Modelled	Actual	Comment	Reference
A	674	ASP	ASN	conflict	UNP A0A386YSI0
A	683	ARG	LYS	conflict	UNP A0A386YSI0
A	687	ILE	MET	conflict	UNP A0A386YSI0
A	691	SER	GLY	conflict	UNP A0A386YSI0
A	693	ILE	VAL	conflict	UNP A0A386YSI0
A	704	LEU	ILE	conflict	UNP A0A386YSI0
A	764	SER	CYS	engineered mutation	UNP A0A386YSI0
A	823	GLY	ALA	engineered mutation	UNP A0A386YSI0
A	837	SER	CYS	engineered mutation	UNP A0A386YSI0
B	674	ASP	ASN	conflict	UNP A0A386YSI0
B	683	ARG	LYS	conflict	UNP A0A386YSI0
B	687	ILE	MET	conflict	UNP A0A386YSI0
B	691	SER	GLY	conflict	UNP A0A386YSI0
B	693	ILE	VAL	conflict	UNP A0A386YSI0
B	704	LEU	ILE	conflict	UNP A0A386YSI0
B	764	SER	CYS	engineered mutation	UNP A0A386YSI0
B	823	GLY	ALA	engineered mutation	UNP A0A386YSI0
B	837	SER	CYS	engineered mutation	UNP A0A386YSI0
C	674	ASP	ASN	conflict	UNP A0A386YSI0
C	683	ARG	LYS	conflict	UNP A0A386YSI0
C	687	ILE	MET	conflict	UNP A0A386YSI0
C	691	SER	GLY	conflict	UNP A0A386YSI0
C	693	ILE	VAL	conflict	UNP A0A386YSI0
C	704	LEU	ILE	conflict	UNP A0A386YSI0
C	764	SER	CYS	engineered mutation	UNP A0A386YSI0
C	823	GLY	ALA	engineered mutation	UNP A0A386YSI0
C	837	SER	CYS	engineered mutation	UNP A0A386YSI0

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

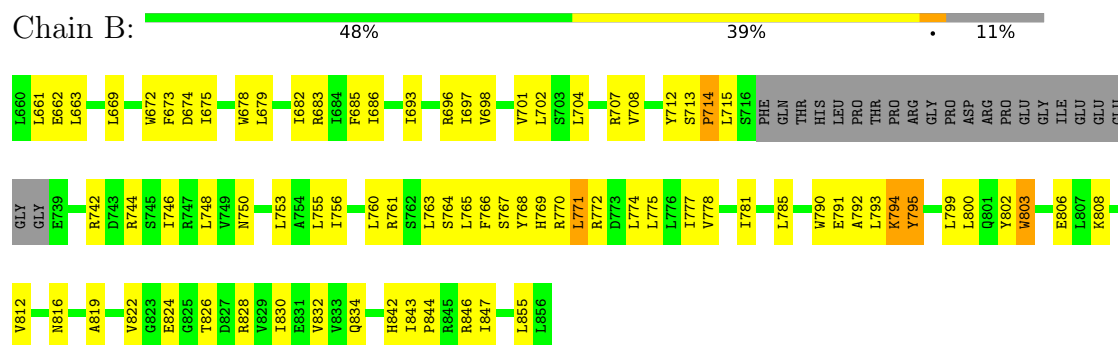
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

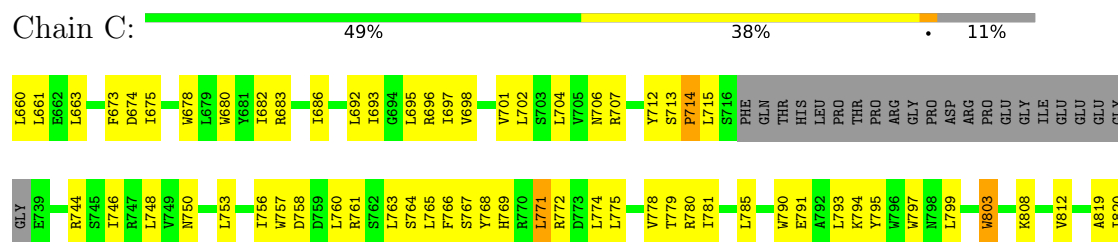
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41



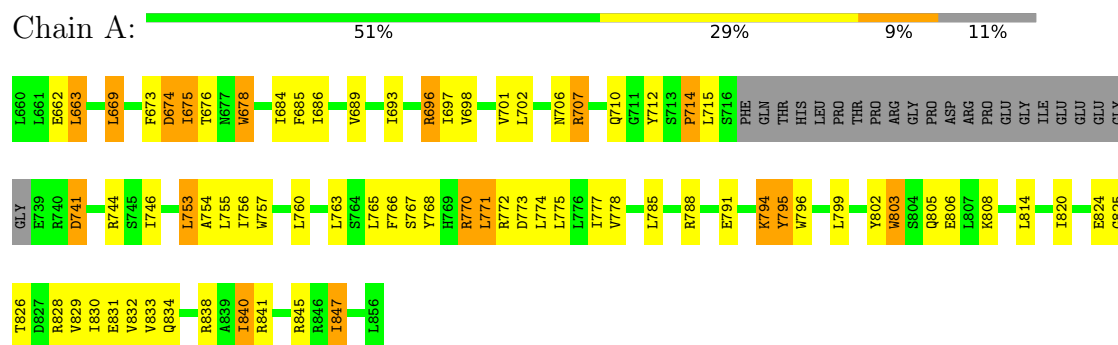


## 4.2 Scores per residue for each member of the ensemble

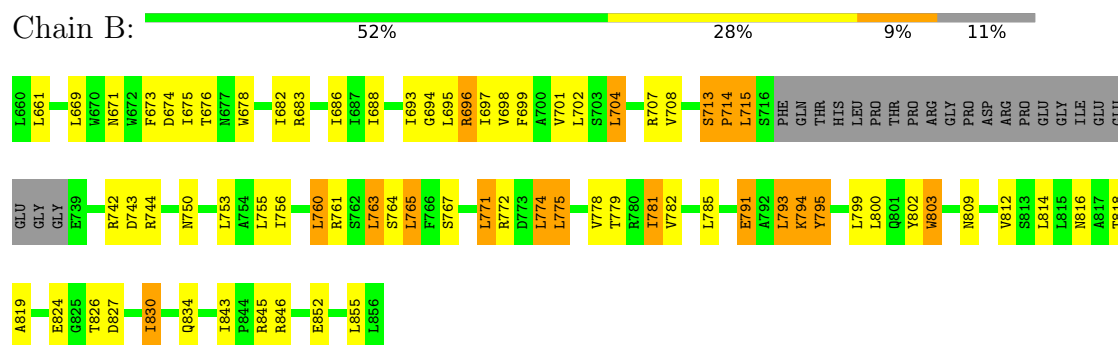
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

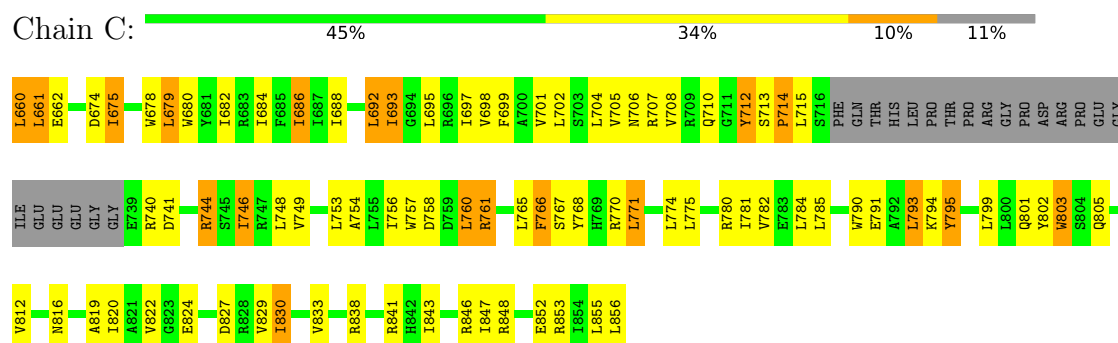
- Molecule 1: Transmembrane protein gp41



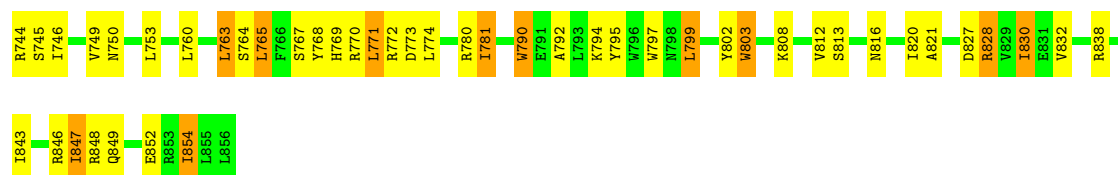
- Molecule 1: Transmembrane protein gp41



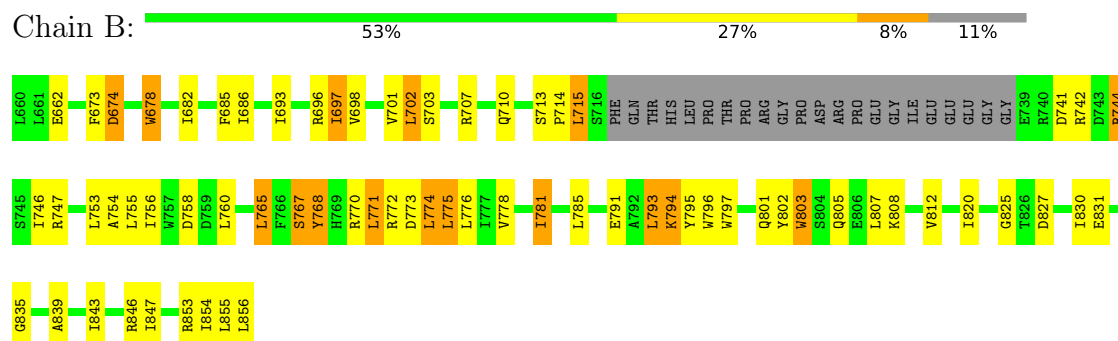
- Molecule 1: Transmembrane protein gp41







#### • Molecule 1: Transmembrane protein gp41

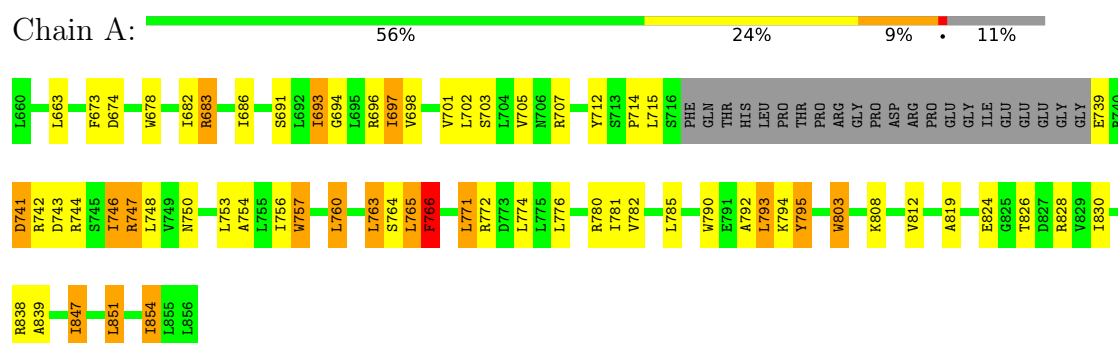


#### • Molecule 1: Transmembrane protein gp41



### 4.2.4 Score per residue for model 4 (medoid)

#### • Molecule 1: Transmembrane protein gp41



#### • Molecule 1: Transmembrane protein gp41

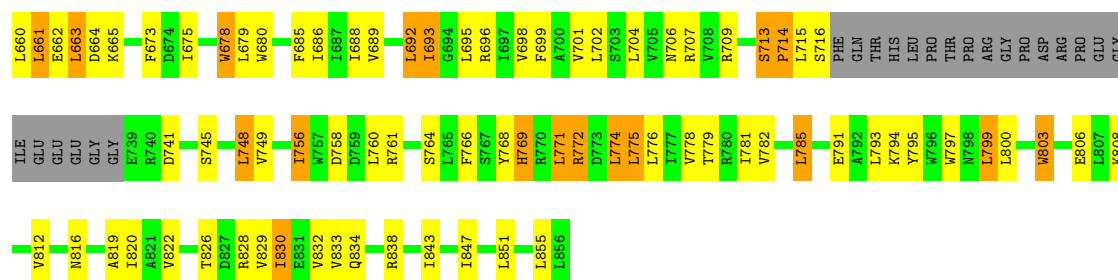






### • Molecule 1: Transmembrane protein gp41

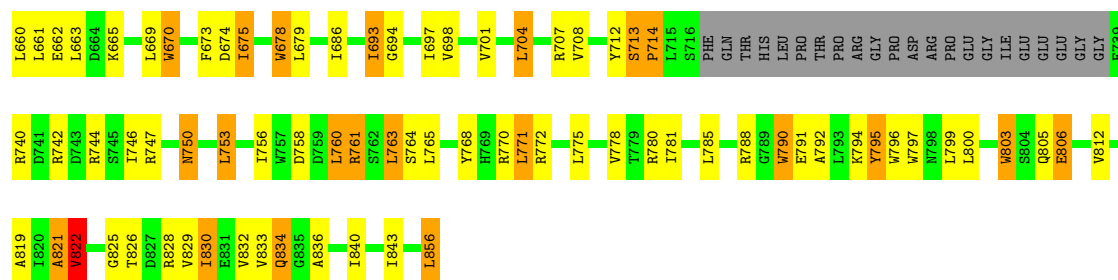
Chain C: 48% 31% 9% 11%



## 4.2.5 Score per residue for model 5

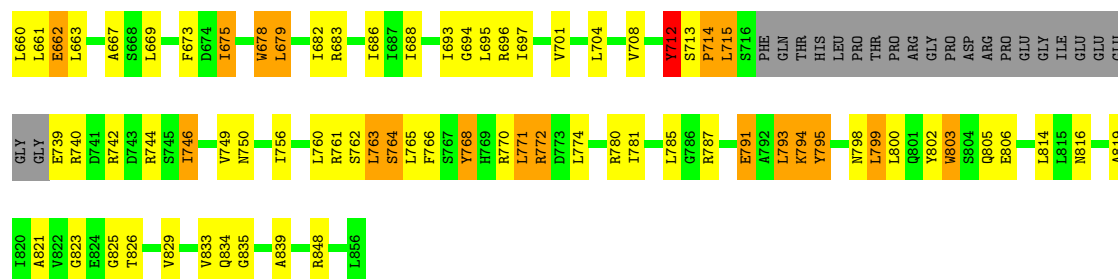
### • Molecule 1: Transmembrane protein gp41

Chain A: 50% 27% 11% • 11%

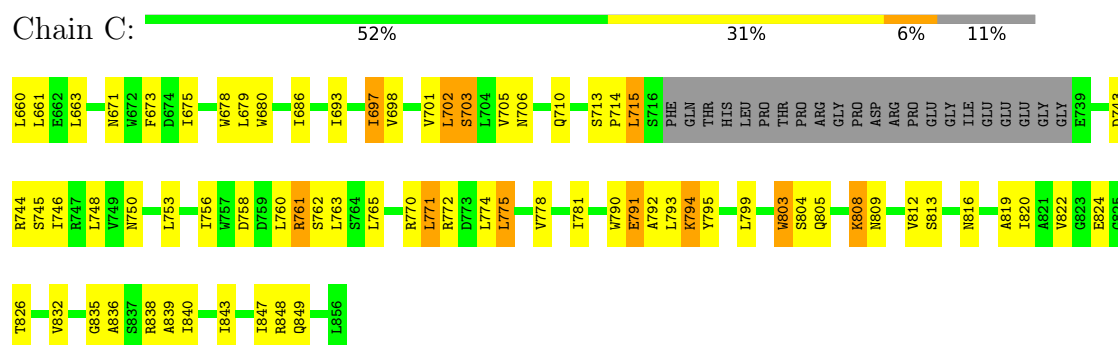


### • Molecule 1: Transmembrane protein gp41

Chain B: 51% 28% 9% • 11%

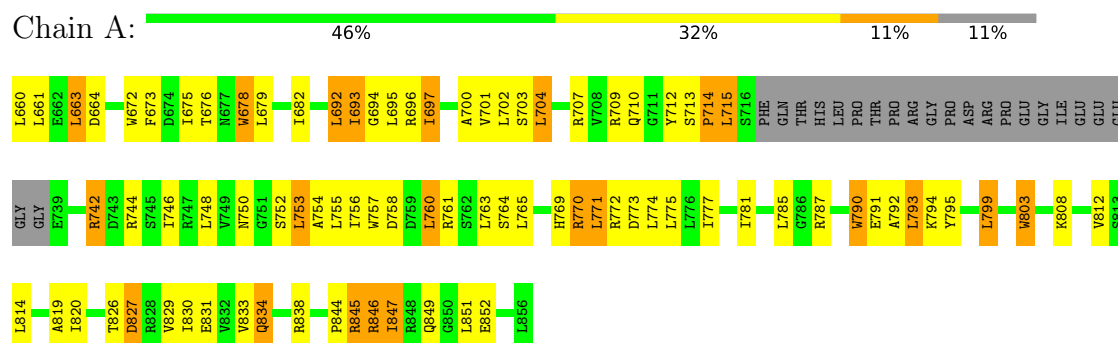


- Molecule 1: Transmembrane protein gp41

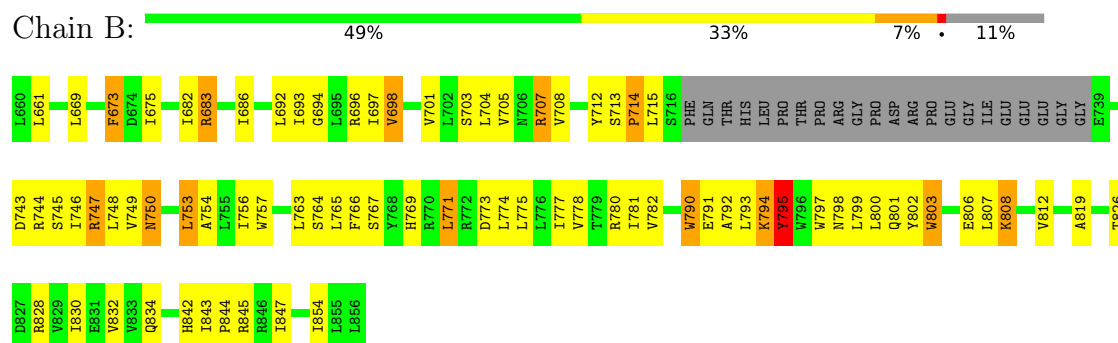


#### 4.2.6 Score per residue for model 6

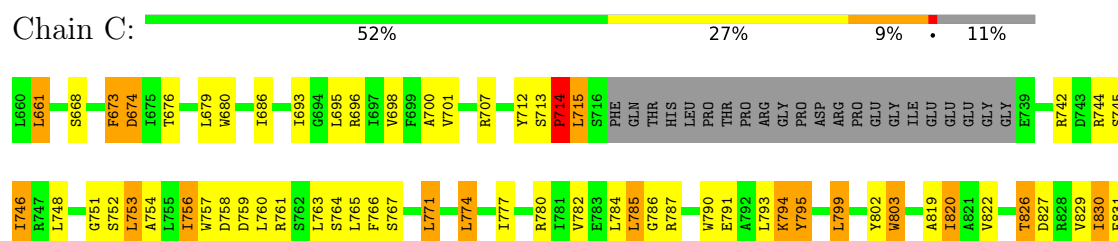
- Molecule 1: Transmembrane protein gp41

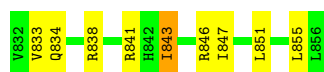


- Molecule 1: Transmembrane protein gp41



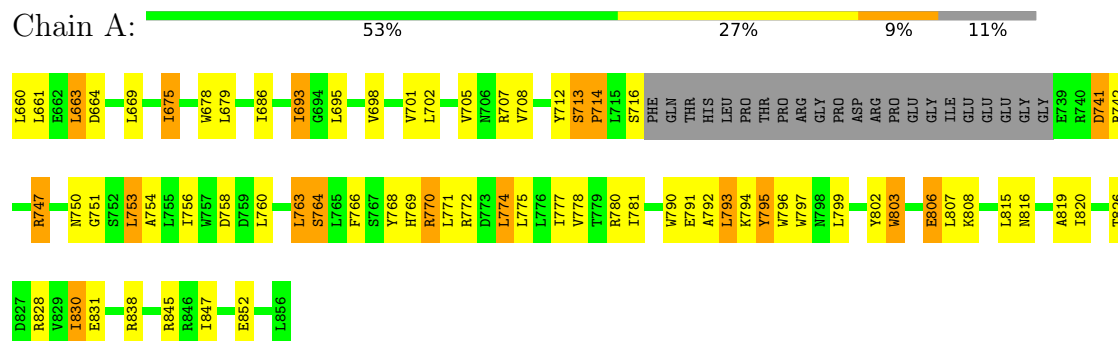
- Molecule 1: Transmembrane protein gp41



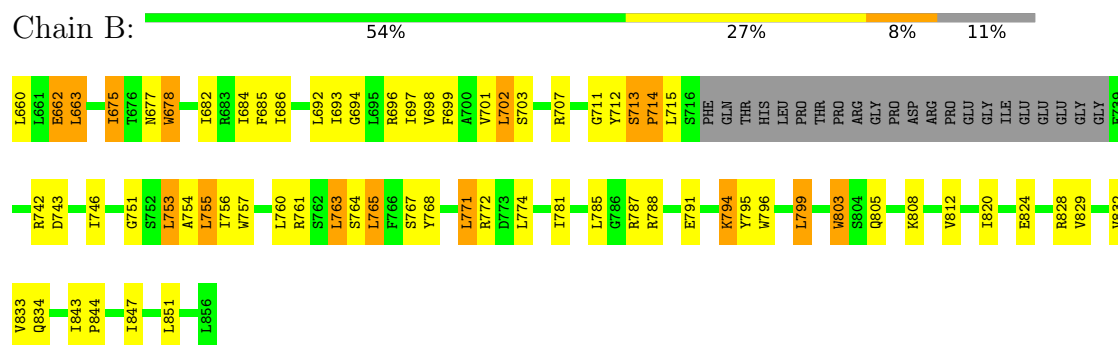


#### 4.2.7 Score per residue for model 7

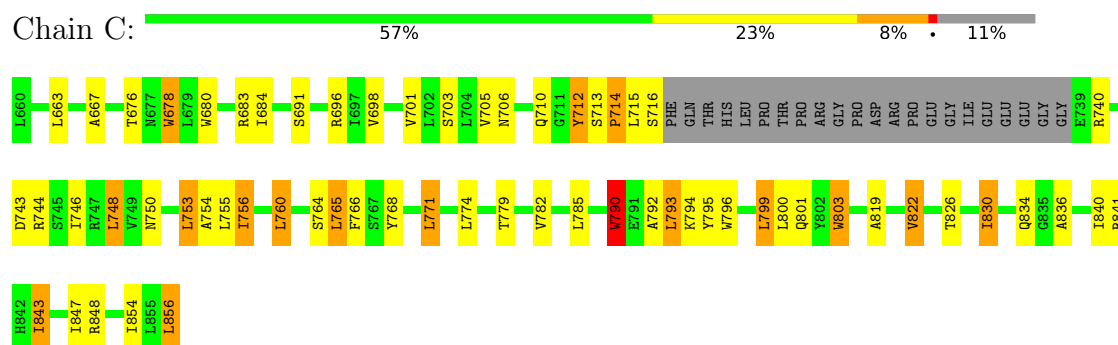
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

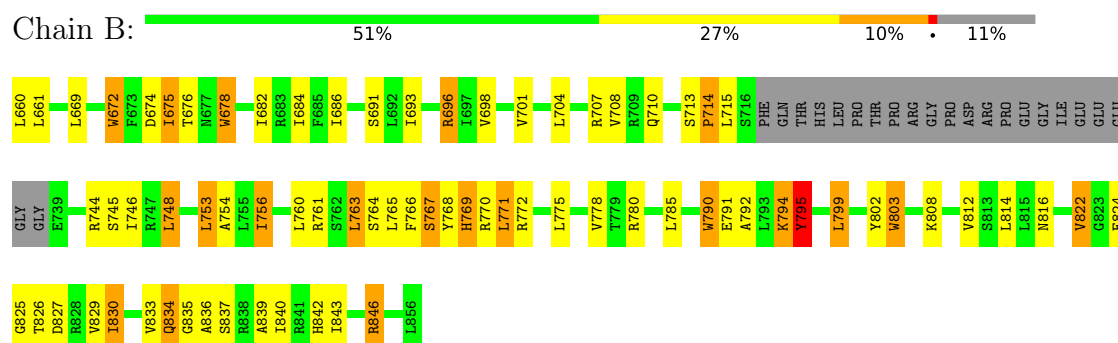
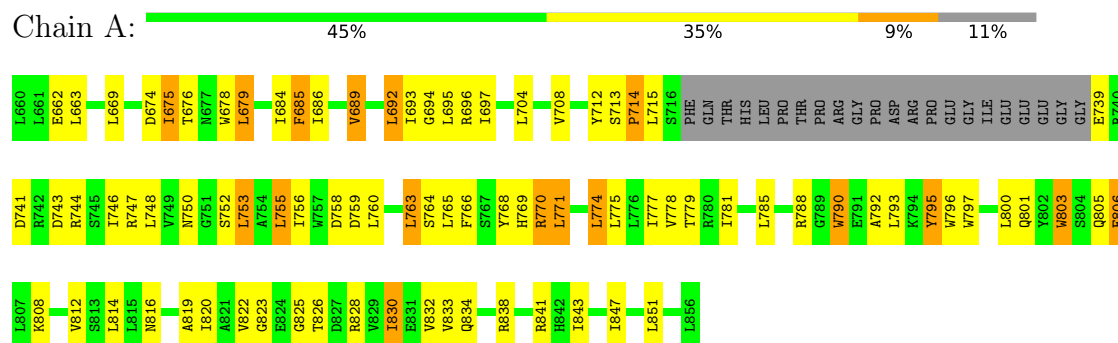


- Molecule 1: Transmembrane protein gp41



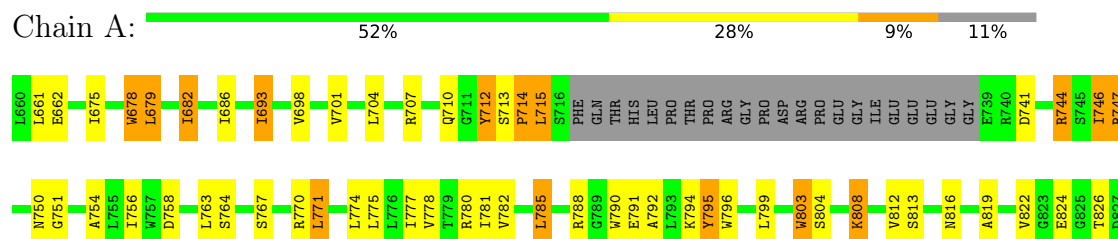
#### 4.2.8 Score per residue for model 8

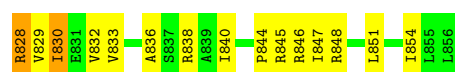
- Molecule 1: Transmembrane protein gp41



#### 4.2.9 Score per residue for model 9

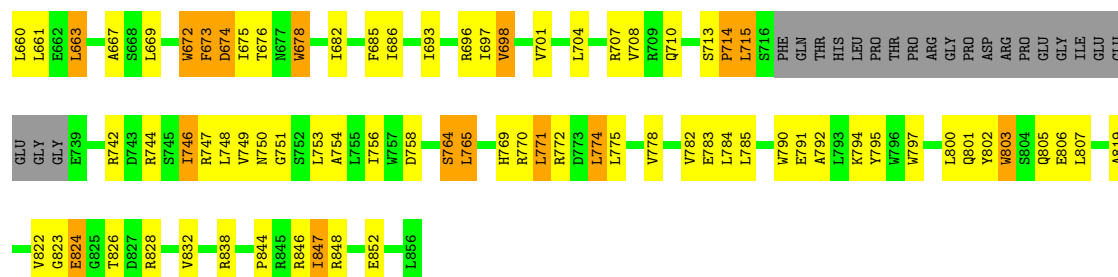
- Molecule 1: Transmembrane protein gp41





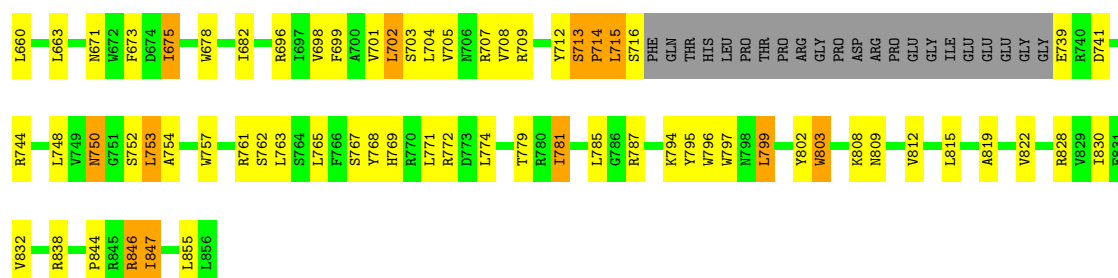
• Molecule 1: Transmembrane protein gp41

Chain B: 50% 31% 8% 11%



• Molecule 1: Transmembrane protein gp41

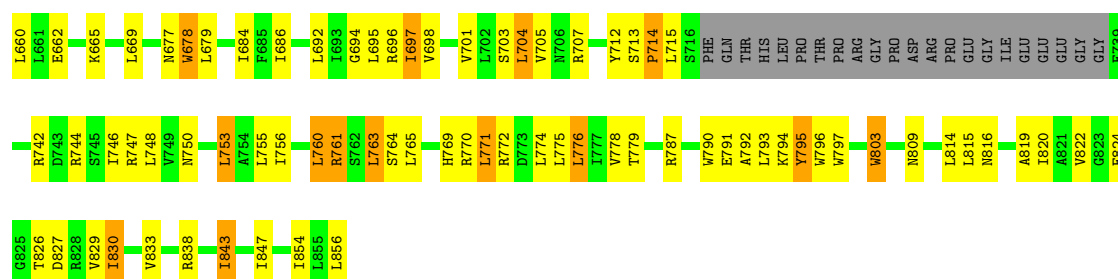
Chain C: 55% 28% 6% 11%



#### 4.2.10 Score per residue for model 10

• Molecule 1: Transmembrane protein gp41

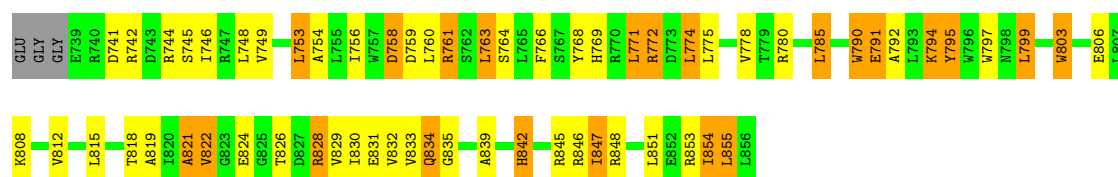
Chain A: 51% 31% 7% 11%



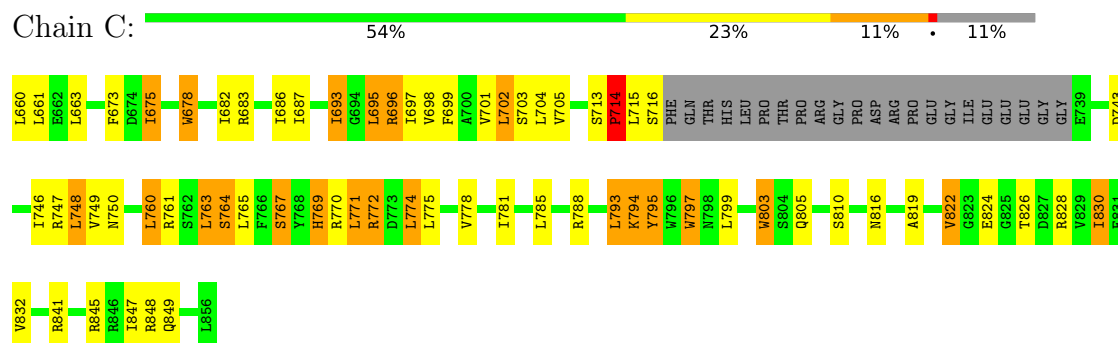
• Molecule 1: Transmembrane protein gp41

Chain B: 43% 32% 14% 11%



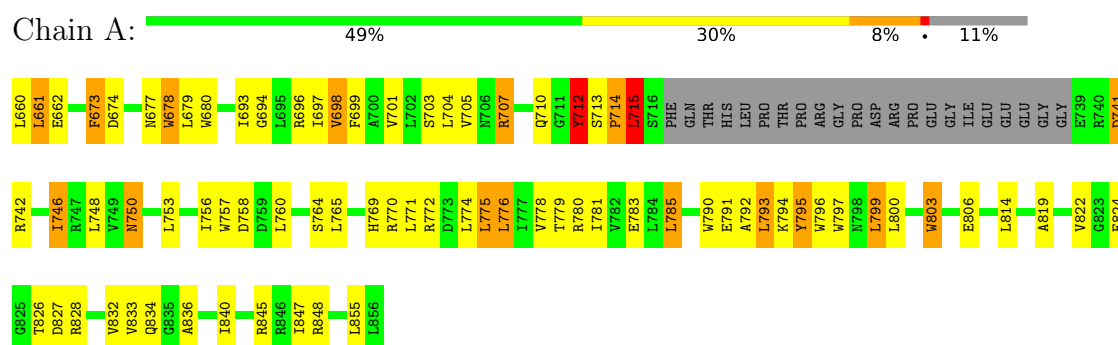


#### • Molecule 1: Transmembrane protein gp41

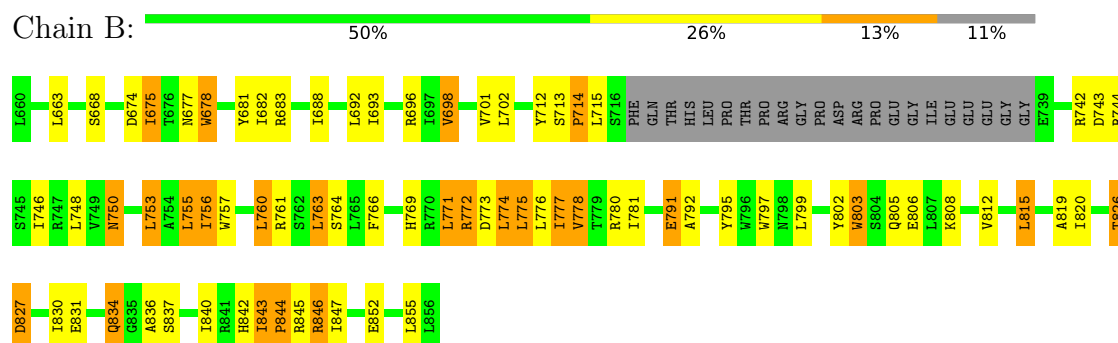


### 4.2.11 Score per residue for model 11

#### • Molecule 1: Transmembrane protein gp41



#### • Molecule 1: Transmembrane protein gp41



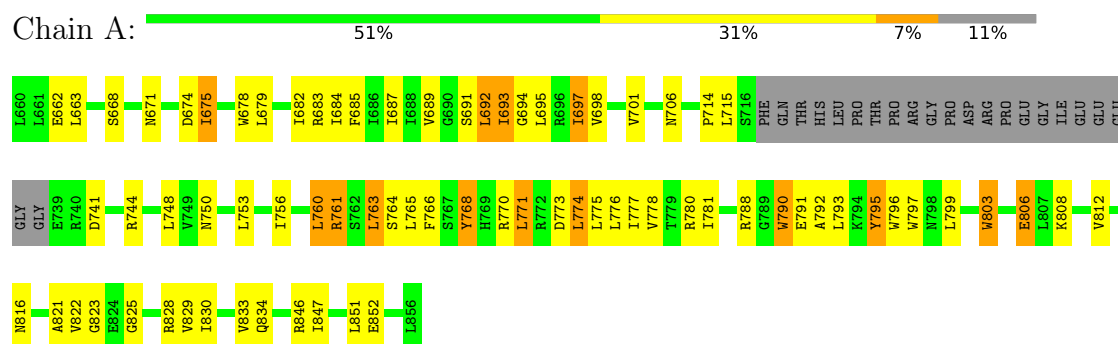
#### • Molecule 1: Transmembrane protein gp41



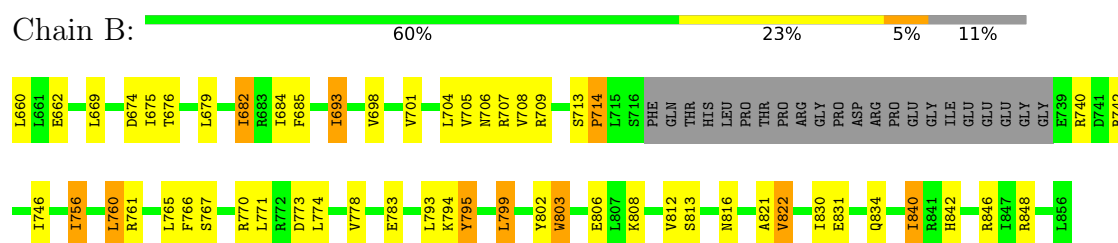


### 4.2.13 Score per residue for model 13

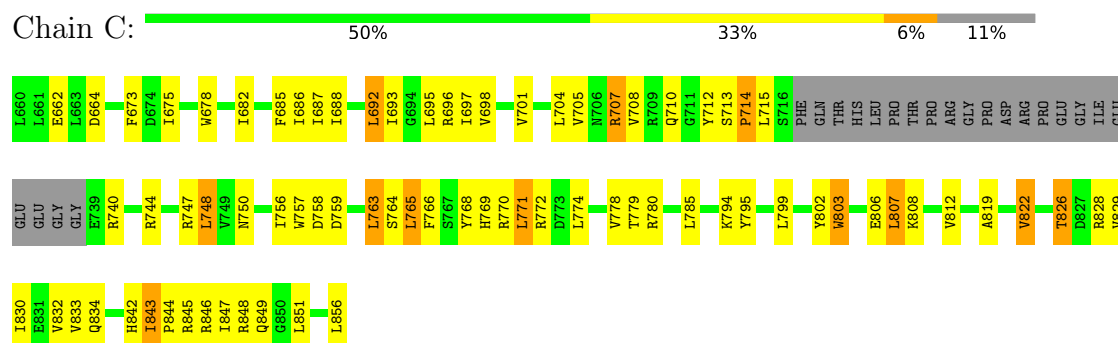
#### • Molecule 1: Transmembrane protein gp41



#### • Molecule 1: Transmembrane protein gp41

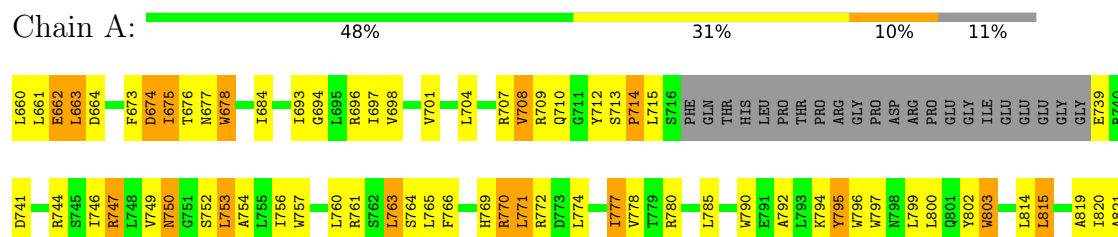


#### • Molecule 1: Transmembrane protein gp41

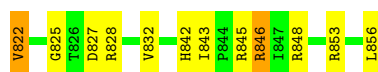


### 4.2.14 Score per residue for model 14

#### • Molecule 1: Transmembrane protein gp41

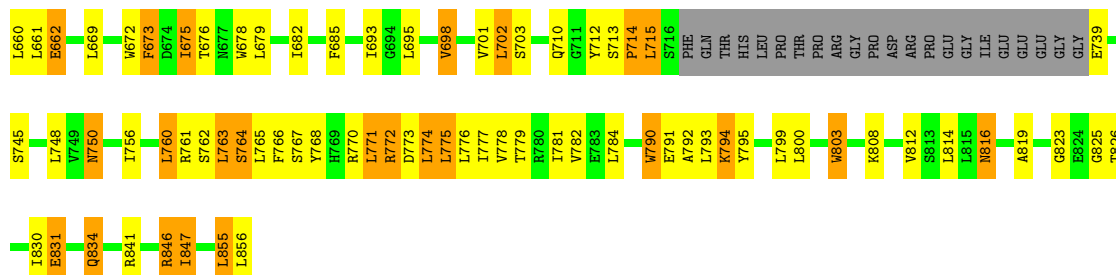






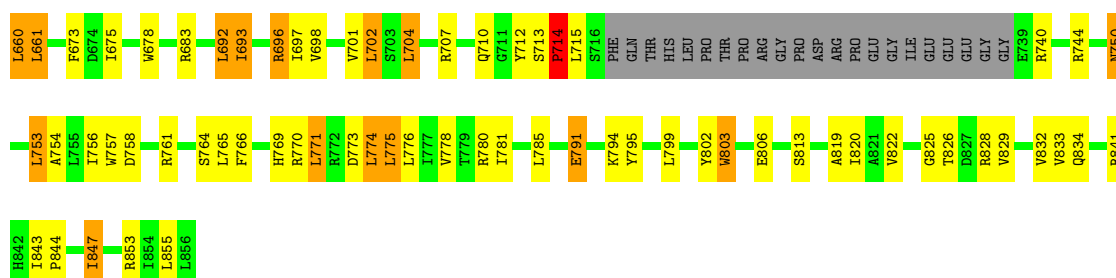
• Molecule 1: Transmembrane protein gp41

Chain B: 51% 26% 12% 11%



• Molecule 1: Transmembrane protein gp41

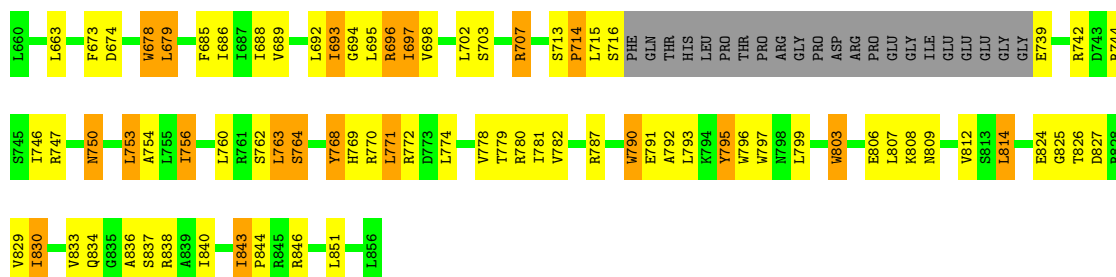
Chain C: 55% 26% 8% 11%



#### 4.2.15 Score per residue for model 15

• Molecule 1: Transmembrane protein gp41

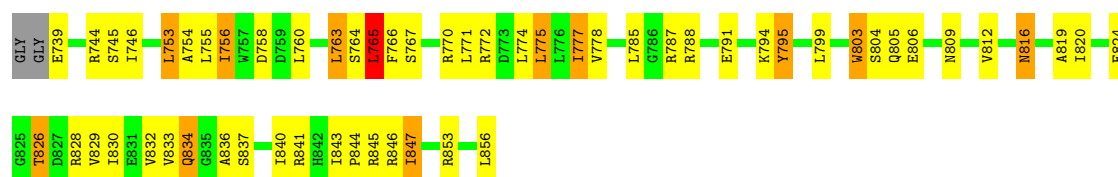
Chain A: 49% 30% 10% 11%



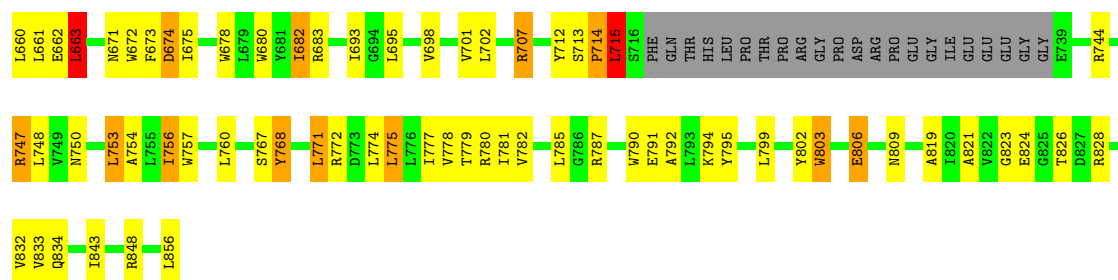
• Molecule 1: Transmembrane protein gp41

Chain B: 47% 33% 9% 11%





• Molecule 1: Transmembrane protein gp41



## 5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

## 6 Model quality i

### 6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.79±0.01	0±0/1490 ( 0.0± 0.0%)	0.97±0.01	0±1/2021 ( 0.0± 0.0%)
1	B	0.79±0.01	0±0/1490 ( 0.0± 0.0%)	0.96±0.01	0±1/2021 ( 0.0± 0.0%)
1	C	0.79±0.01	0±0/1490 ( 0.0± 0.0%)	0.96±0.01	0±0/2021 ( 0.0± 0.0%)
All	All	0.79	0/67050 ( 0.0%)	0.97	12/90945 ( 0.0%)

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

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	795	TYR	CB-CG-CD1	-7.20	116.68	121.00	4	1
1	B	795	TYR	CB-CG-CD1	-6.27	117.24	121.00	6	1
1	A	707	ARG	NE-CZ-NH2	5.66	123.13	120.30	1	2
1	A	685	PHE	CB-CG-CD2	-5.65	116.85	120.80	15	1
1	C	790	TRP	CD1-NE1-CE2	5.44	113.89	109.00	7	1
1	B	712	TYR	CB-CG-CD2	-5.33	117.80	121.00	5	1
1	B	795	TYR	CB-CG-CD2	-5.29	117.83	121.00	8	2
1	C	761	ARG	NE-CZ-NH2	5.11	122.85	120.30	5	1
1	A	795	TYR	CB-CG-CD2	5.09	124.05	121.00	4	1
1	C	696	ARG	NE-CZ-NH2	5.01	122.80	120.30	14	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	770	ARG	Sidechain	1

## 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	1459	1521	1515	55±5
1	B	1459	1521	1515	52±8
1	C	1459	1521	1515	48±6
All	All	65655	68445	68175	1955

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:746:ILE:HG23	1:C:781:ILE:HD12	1.00	1.27	11	1
1:C:819:ALA:HB3	1:C:826:THR:HG21	0.97	1.35	14	1
1:B:819:ALA:HB1	1:B:826:THR:HG23	0.90	1.41	1	1
1:A:686:ILE:HD11	1:C:686:ILE:HG21	0.90	1.43	4	4
1:B:669:LEU:HD13	1:B:676:THR:HG21	0.89	1.43	8	1
1:A:781:ILE:HG21	1:B:746:ILE:HG23	0.84	1.46	9	2
1:A:663:LEU:HD21	1:B:660:LEU:HD23	0.83	1.49	13	1
1:A:686:ILE:HG21	1:B:686:ILE:HD12	0.82	1.50	9	1
1:A:753:LEU:HD13	1:A:754:ALA:N	0.82	1.89	14	5
1:C:695:LEU:O	1:C:698:VAL:HG22	0.79	1.78	12	1
1:B:774:LEU:HD13	1:B:777:ILE:HD12	0.79	1.52	6	2
1:A:799:LEU:HD13	1:B:756:ILE:HD11	0.78	1.54	14	2
1:A:763:LEU:HD23	1:A:764:SER:N	0.78	1.93	5	4
1:C:753:LEU:HD13	1:C:754:ALA:N	0.76	1.93	7	4
1:A:760:LEU:HD13	1:A:761:ARG:N	0.76	1.96	12	4
1:C:713:SER:O	1:C:714:PRO:O	0.75	2.04	11	10
1:C:775:LEU:HD13	1:C:776:LEU:N	0.75	1.96	11	2
1:B:698:VAL:O	1:B:701:VAL:HG22	0.74	1.82	15	13
1:C:715:LEU:HD13	1:C:716:SER:N	0.74	1.97	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:763:LEU:HD22	1:A:764:SER:N	0.74	1.97	12	8
1:B:771:LEU:HD23	1:B:772:ARG:N	0.74	1.98	14	2
1:C:678:TRP:O	1:C:682:ILE:HD12	0.73	1.83	8	1
1:A:819:ALA:O	1:A:822:VAL:HG12	0.73	1.83	10	1
1:A:698:VAL:O	1:A:701:VAL:HG22	0.73	1.84	12	11
1:C:698:VAL:O	1:C:701:VAL:HG22	0.73	1.84	2	13
1:A:713:SER:O	1:A:714:PRO:O	0.73	2.06	7	8
1:C:715:LEU:HD13	1:C:715:LEU:O	0.73	1.83	7	2
1:A:819:ALA:HB3	1:A:827:ASP:OD2	0.72	1.84	10	1
1:C:819:ALA:O	1:C:822:VAL:HG22	0.72	1.84	9	7
1:C:771:LEU:HD22	1:C:772:ARG:N	0.72	1.99	10	1
1:B:771:LEU:HD22	1:B:772:ARG:N	0.72	1.98	5	1
1:A:705:VAL:HG11	1:A:748:LEU:HD12	0.72	1.60	11	1
1:C:774:LEU:HD13	1:C:775:LEU:N	0.72	1.99	12	1
1:C:753:LEU:HD13	1:C:754:ALA:H	0.72	1.45	7	3
1:B:777:ILE:HD12	1:B:778:VAL:N	0.72	2.00	14	1
1:B:763:LEU:O	1:B:774:LEU:HD13	0.71	1.84	1	1
1:B:822:VAL:HG12	1:B:826:THR:HG22	0.71	1.60	8	1
1:C:704:LEU:O	1:C:708:VAL:HG23	0.71	1.85	13	4
1:B:795:TYR:CG	1:C:756:ILE:HG21	0.71	2.21	15	2
1:A:750:ASN:ND2	1:C:785:LEU:HD22	0.71	2.01	3	3
1:B:763:LEU:HD22	1:B:764:SER:N	0.71	2.01	12	6
1:B:795:TYR:CD2	1:C:756:ILE:HG21	0.71	2.21	15	1
1:A:746:ILE:HG21	1:C:781:ILE:CG2	0.71	2.15	1	4
1:B:764:SER:CB	1:B:771:LEU:HD12	0.71	2.16	10	3
1:B:781:ILE:CG2	1:C:746:ILE:HG21	0.71	2.16	12	2
1:C:748:LEU:HD13	1:C:749:VAL:N	0.70	2.01	4	2
1:A:693:ILE:HD13	1:A:694:GLY:N	0.70	2.01	3	1
1:B:777:ILE:HD13	1:B:778:VAL:N	0.70	2.01	12	3
1:B:763:LEU:O	1:B:774:LEU:HD21	0.70	1.87	2	1
1:A:707:ARG:CB	1:C:704:LEU:HD11	0.70	2.16	4	1
1:C:663:LEU:HD13	1:C:664:ASP:N	0.70	2.02	4	3
1:A:764:SER:CB	1:A:771:LEU:HD22	0.70	2.16	13	1
1:A:746:ILE:HG21	1:C:781:ILE:HG23	0.69	1.64	15	3
1:B:760:LEU:O	1:B:760:LEU:HD22	0.69	1.87	11	7
1:A:771:LEU:HD22	1:A:772:ARG:N	0.69	2.02	15	1
1:A:819:ALA:HB1	1:A:826:THR:CG2	0.69	2.17	9	1
1:B:667:ALA:HB2	1:C:660:LEU:HD11	0.69	1.63	2	1
1:B:715:LEU:HD12	1:B:716:SER:N	0.69	2.02	4	1
1:B:715:LEU:HD22	1:B:715:LEU:O	0.69	1.87	9	2
1:B:797:TRP:CG	1:B:847:ILE:HD11	0.69	2.23	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:777:ILE:HD13	1:A:778:VAL:N	0.69	2.03	14	1
1:A:756:ILE:HD11	1:C:796:TRP:CD1	0.69	2.22	7	1
1:B:751:GLY:O	1:C:715:LEU:HD12	0.69	1.87	7	1
1:B:795:TYR:CB	1:C:756:ILE:HG21	0.69	2.18	14	2
1:A:685:PHE:O	1:A:689:VAL:HG22	0.69	1.88	8	1
1:A:799:LEU:CD1	1:B:756:ILE:HD11	0.69	2.18	14	1
1:C:771:LEU:HD13	1:C:772:ARG:H	0.69	1.47	4	1
1:B:713:SER:O	1:B:714:PRO:O	0.68	2.11	10	11
1:B:760:LEU:HD13	1:B:761:ARG:N	0.68	2.04	14	5
1:C:771:LEU:H	1:C:771:LEU:HD23	0.68	1.47	15	2
1:A:715:LEU:O	1:A:715:LEU:HD13	0.68	1.89	15	3
1:C:819:ALA:O	1:C:822:VAL:HG12	0.68	1.89	11	3
1:A:781:ILE:HD13	1:B:746:ILE:CG1	0.68	2.17	3	1
1:A:781:ILE:HG21	1:B:746:ILE:CG2	0.68	2.17	9	3
1:A:660:LEU:O	1:C:663:LEU:HD22	0.68	1.87	5	1
1:A:771:LEU:H	1:A:771:LEU:HD13	0.68	1.48	15	8
1:B:753:LEU:HD13	1:B:754:ALA:N	0.68	2.04	7	2
1:C:763:LEU:HD22	1:C:764:SER:N	0.68	2.04	10	1
1:A:756:ILE:O	1:A:760:LEU:HD12	0.68	1.88	12	3
1:A:685:PHE:O	1:A:689:VAL:HG23	0.68	1.88	1	3
1:B:751:GLY:CA	1:C:715:LEU:HD11	0.68	2.19	2	1
1:B:669:LEU:HD13	1:B:669:LEU:O	0.67	1.89	1	2
1:B:686:ILE:HG21	1:C:686:ILE:HD11	0.67	1.67	2	2
1:A:757:TRP:CZ3	1:B:715:LEU:HD13	0.67	2.24	4	1
1:B:775:LEU:O	1:B:775:LEU:HD22	0.67	1.89	11	2
1:B:803:TRP:CH2	1:C:760:LEU:HD22	0.67	2.23	4	1
1:B:852:GLU:O	1:B:855:LEU:HD12	0.67	1.90	2	1
1:A:693:ILE:HD11	1:B:696:ARG:NE	0.67	2.05	7	5
1:A:746:ILE:HG23	1:C:781:ILE:CD1	0.67	2.12	11	1
1:A:694:GLY:O	1:A:697:ILE:HD12	0.67	1.89	3	3
1:C:748:LEU:HD22	1:C:748:LEU:O	0.67	1.90	8	2
1:B:669:LEU:CD1	1:B:676:THR:HG21	0.67	2.20	8	1
1:B:704:LEU:HD11	1:C:707:ARG:CB	0.67	2.20	2	1
1:B:682:ILE:HD12	1:B:683:ARG:N	0.67	2.04	1	6
1:B:775:LEU:O	1:B:778:VAL:HG22	0.67	1.90	6	5
1:B:781:ILE:HG23	1:C:746:ILE:HG21	0.67	1.67	12	1
1:A:753:LEU:HD22	1:A:753:LEU:C	0.66	2.11	6	4
1:C:702:LEU:HD22	1:C:702:LEU:O	0.66	1.90	12	3
1:C:830:ILE:H	1:C:830:ILE:HD13	0.66	1.49	6	1
1:A:756:ILE:HD13	1:C:796:TRP:NE1	0.66	2.05	9	1
1:B:750:ASN:O	1:B:753:LEU:HD12	0.66	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:678:TRP:O	1:B:682:ILE:HG23	0.66	1.90	1	8
1:B:704:LEU:O	1:B:708:VAL:HG23	0.66	1.90	15	3
1:A:705:VAL:HG21	1:A:748:LEU:HD12	0.66	1.68	10	2
1:A:675:ILE:HD13	1:A:675:ILE:O	0.66	1.90	7	4
1:C:797:TRP:CD1	1:C:847:ILE:HD11	0.66	2.25	12	2
1:C:774:LEU:O	1:C:774:LEU:HD22	0.66	1.91	12	1
1:A:682:ILE:HD12	1:A:683:ARG:N	0.66	2.06	4	1
1:B:793:LEU:HD13	1:B:793:LEU:O	0.66	1.91	13	4
1:B:785:LEU:HD23	1:C:750:ASN:OD1	0.66	1.89	5	1
1:B:779:THR:O	1:B:782:VAL:HG22	0.65	1.91	14	2
1:B:795:TYR:HB3	1:C:756:ILE:HG21	0.65	1.67	14	2
1:A:791:GLU:O	1:A:794:LYS:HG3	0.65	1.91	12	1
1:C:760:LEU:HD22	1:C:760:LEU:O	0.65	1.91	1	1
1:A:785:LEU:HD13	1:A:785:LEU:O	0.65	1.90	14	3
1:A:803:TRP:CH2	1:B:760:LEU:HD23	0.65	2.26	13	1
1:B:781:ILE:HD12	1:B:782:VAL:N	0.65	2.07	6	1
1:A:663:LEU:HD22	1:A:663:LEU:O	0.65	1.90	14	1
1:A:819:ALA:O	1:A:826:THR:HG21	0.65	1.91	2	2
1:B:753:LEU:HD22	1:B:754:ALA:N	0.65	2.07	6	1
1:A:802:TYR:CD1	1:B:760:LEU:HD21	0.65	2.26	7	1
1:A:829:VAL:O	1:A:833:VAL:HG22	0.65	1.91	1	6
1:A:754:ALA:CB	1:B:715:LEU:HD11	0.65	2.21	4	1
1:B:675:ILE:HD13	1:B:675:ILE:O	0.65	1.92	8	2
1:A:776:LEU:HD13	1:A:776:LEU:H	0.65	1.51	10	1
1:C:695:LEU:HD22	1:C:695:LEU:C	0.65	2.12	10	1
1:C:746:ILE:O	1:C:749:VAL:HG22	0.64	1.92	8	2
1:B:755:LEU:HD13	1:B:755:LEU:O	0.64	1.93	7	2
1:A:663:LEU:HD12	1:A:664:ASP:N	0.64	2.07	12	1
1:A:763:LEU:HD23	1:A:764:SER:H	0.64	1.52	8	1
1:B:702:LEU:O	1:B:702:LEU:HD22	0.64	1.92	14	3
1:A:755:LEU:HD13	1:A:756:ILE:N	0.64	2.06	8	1
1:A:750:ASN:OD1	1:C:785:LEU:HD23	0.64	1.91	10	1
1:A:715:LEU:HD12	1:C:754:ALA:O	0.64	1.92	15	1
1:A:753:LEU:HD23	1:C:791:GLU:HB3	0.64	1.67	6	3
1:B:702:LEU:C	1:B:702:LEU:HD13	0.64	2.13	2	5
1:A:763:LEU:H	1:A:763:LEU:HD13	0.64	1.50	4	8
1:A:775:LEU:O	1:A:778:VAL:HG12	0.64	1.91	5	7
1:A:854:ILE:O	1:A:854:ILE:HD13	0.64	1.92	4	2
1:A:816:ASN:N	1:A:830:ILE:HD11	0.64	2.06	13	2
1:B:669:LEU:HD11	1:B:675:ILE:HG23	0.64	1.69	9	1
1:C:764:SER:OG	1:C:771:LEU:HD12	0.64	1.92	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:822:VAL:HG21	1:C:826:THR:HG21	0.64	1.69	8	1
1:C:775:LEU:O	1:C:778:VAL:HG22	0.64	1.93	4	4
1:B:855:LEU:HD22	1:B:855:LEU:O	0.63	1.93	2	2
1:A:799:LEU:O	1:A:803:TRP:CE3	0.63	2.51	3	4
1:C:799:LEU:HD23	1:C:800:LEU:N	0.63	2.08	3	1
1:C:771:LEU:H	1:C:771:LEU:HD13	0.63	1.52	10	7
1:A:774:LEU:O	1:A:777:ILE:HG22	0.63	1.92	6	1
1:C:797:TRP:NE1	1:C:847:ILE:HD11	0.63	2.08	9	1
1:C:692:LEU:HD23	1:C:693:ILE:N	0.63	2.07	14	1
1:A:715:LEU:HD12	1:C:751:GLY:CA	0.63	2.23	2	1
1:A:750:ASN:ND2	1:C:785:LEU:HD23	0.63	2.09	2	6
1:A:756:ILE:CG2	1:A:760:LEU:HD12	0.63	2.22	6	1
1:B:764:SER:HB3	1:B:771:LEU:HD12	0.63	1.70	7	4
1:A:755:LEU:HD22	1:A:755:LEU:O	0.63	1.93	8	1
1:B:799:LEU:HD23	1:B:800:LEU:N	0.63	2.08	2	1
1:A:756:ILE:HD13	1:C:795:TYR:HB3	0.63	1.68	10	2
1:C:768:TYR:CD2	1:C:771:LEU:HD11	0.63	2.28	13	1
1:C:675:ILE:O	1:C:675:ILE:HD13	0.63	1.94	10	3
1:B:785:LEU:HD23	1:C:750:ASN:ND2	0.63	2.09	15	2
1:C:678:TRP:O	1:C:682:ILE:HG23	0.63	1.94	15	2
1:C:819:ALA:HB1	1:C:826:THR:CG2	0.63	2.23	11	1
1:B:756:ILE:HD13	1:B:756:ILE:O	0.63	1.93	2	2
1:C:828:ARG:O	1:C:832:VAL:HG23	0.63	1.94	13	4
1:C:776:LEU:O	1:C:779:THR:HG22	0.63	1.94	4	2
1:B:686:ILE:HG21	1:C:686:ILE:CD1	0.63	2.24	5	1
1:A:760:LEU:O	1:A:763:LEU:HD22	0.62	1.94	4	1
1:A:793:LEU:HD21	1:A:847:ILE:HG12	0.62	1.72	4	1
1:A:806:GLU:CB	1:B:771:LEU:HD21	0.62	2.23	8	2
1:C:816:ASN:OD1	1:C:830:ILE:HD12	0.62	1.94	1	2
1:B:702:LEU:HD13	1:B:703:SER:N	0.62	2.09	7	4
1:C:816:ASN:O	1:C:820:ILE:HD12	0.62	1.94	5	2
1:C:826:THR:O	1:C:829:VAL:HG12	0.62	1.94	8	3
1:C:675:ILE:HG22	1:C:679:LEU:CD1	0.62	2.25	4	1
1:A:747:ARG:NH1	1:A:754:ALA:HB2	0.62	2.09	7	1
1:A:806:GLU:HB3	1:B:771:LEU:HD11	0.62	1.72	13	1
1:A:797:TRP:CD1	1:A:847:ILE:HD11	0.62	2.29	3	1
1:B:806:GLU:CD	1:C:771:LEU:HD21	0.62	2.14	12	1
1:C:708:VAL:HG12	1:C:741:ASP:OD2	0.62	1.94	1	1
1:C:748:LEU:HD13	1:C:748:LEU:O	0.62	1.92	11	5
1:B:795:TYR:HB3	1:C:756:ILE:HD13	0.62	1.71	6	1
1:A:770:ARG:NH1	1:A:777:ILE:HD13	0.62	2.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:835:GLY:O	1:B:839:ALA:HB3	0.62	1.94	4	7
1:C:685:PHE:HA	1:C:688:ILE:HD12	0.62	1.71	13	2
1:A:669:LEU:CD2	1:A:676:THR:HG23	0.62	2.24	8	1
1:B:669:LEU:CD2	1:B:676:THR:HG23	0.62	2.25	9	1
1:B:826:THR:O	1:B:830:ILE:HD12	0.62	1.94	15	1
1:A:752:SER:O	1:A:755:LEU:HD12	0.61	1.95	8	1
1:B:800:LEU:HA	1:B:803:TRP:CH2	0.61	2.30	9	1
1:A:781:ILE:HD13	1:B:746:ILE:HG13	0.61	1.72	12	2
1:C:697:ILE:HD13	1:C:697:ILE:O	0.61	1.95	5	1
1:B:663:LEU:HD23	1:B:663:LEU:O	0.61	1.94	10	1
1:C:819:ALA:HB1	1:C:826:THR:OG1	0.61	1.96	10	2
1:A:819:ALA:HB1	1:A:826:THR:OG1	0.61	1.94	12	1
1:B:808:LYS:O	1:B:812:VAL:HG22	0.61	1.96	7	3
1:A:696:ARG:HE	1:C:693:ILE:HD11	0.61	1.56	14	3
1:A:686:ILE:CG2	1:B:686:ILE:HD12	0.61	2.25	9	1
1:B:771:LEU:H	1:B:771:LEU:HD13	0.61	1.55	3	7
1:B:775:LEU:H	1:B:775:LEU:HD13	0.61	1.56	1	3
1:A:714:PRO:HB2	1:C:748:LEU:HD23	0.61	1.71	10	1
1:A:708:VAL:HG21	1:B:714:PRO:HD3	0.61	1.70	2	2
1:C:682:ILE:HD12	1:C:683:ARG:N	0.61	2.10	10	2
1:C:695:LEU:O	1:C:698:VAL:HG13	0.61	1.96	10	1
1:B:819:ALA:HB1	1:B:826:THR:HB	0.61	1.72	2	5
1:B:828:ARG:O	1:B:832:VAL:HG23	0.61	1.96	12	5
1:B:774:LEU:HD23	1:B:775:LEU:N	0.61	2.10	3	1
1:A:816:ASN:CA	1:A:830:ILE:HD11	0.61	2.26	13	3
1:B:704:LEU:HD21	1:C:714:PRO:O	0.61	1.95	1	1
1:A:840:ILE:HD13	1:A:840:ILE:O	0.61	1.94	2	2
1:B:750:ASN:O	1:B:753:LEU:HD13	0.61	1.96	6	1
1:B:854:ILE:HD13	1:B:854:ILE:O	0.60	1.96	10	1
1:A:796:TRP:HE1	1:B:756:ILE:HD13	0.60	1.57	1	1
1:B:685:PHE:O	1:B:689:VAL:HG23	0.60	1.95	12	2
1:B:759:ASP:O	1:B:763:LEU:HD12	0.60	1.95	4	2
1:B:746:ILE:O	1:B:749:VAL:HG22	0.60	1.96	12	3
1:C:756:ILE:O	1:C:756:ILE:HD13	0.60	1.95	15	1
1:B:704:LEU:HD11	1:C:712:TYR:O	0.60	1.96	9	1
1:A:776:LEU:HD13	1:A:776:LEU:N	0.60	2.11	10	1
1:A:781:ILE:HG22	1:B:746:ILE:HG21	0.60	1.73	15	1
1:B:748:LEU:O	1:B:748:LEU:HD13	0.60	1.96	11	1
1:A:764:SER:OG	1:A:771:LEU:HD22	0.60	1.96	13	1
1:A:785:LEU:HD22	1:B:750:ASN:ND2	0.60	2.12	5	1
1:B:663:LEU:O	1:B:667:ALA:HB3	0.60	1.96	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:715:LEU:HD22	1:C:715:LEU:O	0.60	1.96	2	2
1:C:829:VAL:O	1:C:833:VAL:HG22	0.60	1.96	14	3
1:A:785:LEU:HD13	1:B:749:VAL:HB	0.60	1.74	5	1
1:B:753:LEU:HD12	1:B:754:ALA:N	0.60	2.12	10	2
1:B:820:ILE:O	1:B:822:VAL:HG22	0.60	1.97	12	1
1:A:781:ILE:CG2	1:B:746:ILE:HG21	0.60	2.26	15	5
1:A:697:ILE:O	1:A:697:ILE:HD13	0.60	1.97	10	2
1:A:816:ASN:HA	1:A:830:ILE:HD11	0.60	1.70	12	2
1:B:812:VAL:HG11	1:B:834:GLN:NE2	0.60	2.11	10	1
1:B:768:TYR:O	1:B:771:LEU:HD13	0.60	1.96	12	1
1:B:847:ILE:H	1:B:847:ILE:HD13	0.60	1.57	12	1
1:C:693:ILE:HD12	1:C:693:ILE:O	0.60	1.97	4	6
1:C:812:VAL:HG12	1:C:834:GLN:CD	0.60	2.17	8	1
1:B:781:ILE:HG21	1:C:746:ILE:CG2	0.59	2.27	2	2
1:C:763:LEU:O	1:C:774:LEU:HD22	0.59	1.97	6	1
1:A:793:LEU:HD12	1:A:797:TRP:NE1	0.59	2.11	11	2
1:A:753:LEU:HD23	1:C:791:GLU:CB	0.59	2.27	2	3
1:A:754:ALA:HB1	1:B:715:LEU:HB3	0.59	1.73	7	1
1:A:765:LEU:HD12	1:A:770:ARG:NH2	0.59	2.13	1	1
1:A:678:TRP:O	1:A:682:ILE:HG23	0.59	1.96	13	2
1:A:793:LEU:HD12	1:A:847:ILE:HD11	0.59	1.75	7	2
1:C:771:LEU:HD23	1:C:772:ARG:CD	0.59	2.26	11	1
1:C:771:LEU:HD13	1:C:772:ARG:N	0.59	2.12	4	1
1:A:785:LEU:HD21	1:B:746:ILE:HG22	0.59	1.73	5	1
1:A:830:ILE:HD13	1:A:831:GLU:N	0.59	2.12	7	1
1:B:799:LEU:HD22	1:C:756:ILE:HD12	0.59	1.75	8	1
1:C:812:VAL:HG12	1:C:834:GLN:NE2	0.59	2.13	8	1
1:C:715:LEU:C	1:C:715:LEU:HD22	0.59	2.18	9	1
1:A:756:ILE:HG21	1:C:795:TYR:HB3	0.59	1.75	6	3
1:B:694:GLY:O	1:B:697:ILE:HG22	0.59	1.98	5	4
1:B:793:LEU:O	1:B:793:LEU:HD23	0.59	1.98	6	2
1:A:828:ARG:O	1:A:832:VAL:HG22	0.59	1.98	11	2
1:B:760:LEU:C	1:B:760:LEU:HD13	0.59	2.19	3	3
1:A:704:LEU:HD11	1:B:707:ARG:CB	0.58	2.27	2	2
1:A:758:ASP:HB3	1:B:715:LEU:HD11	0.58	1.75	12	1
1:B:840:ILE:HD13	1:B:840:ILE:O	0.58	1.97	2	2
1:C:821:ALA:O	1:C:822:VAL:HG13	0.58	1.97	2	1
1:A:765:LEU:HD13	1:A:766:PHE:N	0.58	2.13	4	1
1:A:799:LEU:HD23	1:A:800:LEU:N	0.58	2.13	11	1
1:A:753:LEU:HD13	1:A:754:ALA:H	0.58	1.58	6	1
1:A:753:LEU:O	1:A:756:ILE:HG22	0.58	1.98	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:791:GLU:O	1:B:794:LYS:HG3	0.58	1.99	6	9
1:B:796:TRP:HE1	1:C:756:ILE:HD11	0.58	1.59	2	1
1:B:702:LEU:O	1:B:702:LEU:HD13	0.58	1.99	4	1
1:B:682:ILE:HD13	1:B:682:ILE:C	0.58	2.18	13	1
1:A:686:ILE:HG21	1:B:686:ILE:CD1	0.58	2.28	9	2
1:B:799:LEU:HD13	1:C:756:ILE:HD11	0.58	1.76	5	1
1:B:799:LEU:O	1:B:803:TRP:CD2	0.58	2.57	13	3
1:B:693:ILE:HD11	1:C:692:LEU:HD23	0.58	1.75	8	3
1:A:663:LEU:HD13	1:A:664:ASP:N	0.58	2.14	14	2
1:A:750:ASN:CG	1:C:785:LEU:HD22	0.58	2.19	9	2
1:C:793:LEU:HD22	1:C:793:LEU:O	0.58	1.99	10	1
1:C:793:LEU:HD21	1:C:797:TRP:NE1	0.58	2.14	10	1
1:A:796:TRP:CD1	1:B:756:ILE:HD13	0.58	2.34	10	2
1:B:793:LEU:HD11	1:B:847:ILE:HG13	0.58	1.74	12	1
1:A:754:ALA:HB1	1:B:715:LEU:O	0.57	1.99	1	2
1:C:774:LEU:HD13	1:C:774:LEU:O	0.57	1.99	14	2
1:C:791:GLU:O	1:C:794:LYS:HG3	0.57	1.99	5	2
1:B:702:LEU:HD13	1:B:702:LEU:C	0.57	2.20	7	1
1:B:669:LEU:HD11	1:B:675:ILE:CG2	0.57	2.28	9	1
1:A:774:LEU:O	1:A:778:VAL:HG23	0.57	1.99	15	1
1:C:708:VAL:HG11	1:C:744:ARG:NH1	0.57	2.13	1	1
1:B:829:VAL:O	1:B:833:VAL:HG23	0.57	1.99	4	4
1:B:855:LEU:HD13	1:B:855:LEU:O	0.57	2.00	14	2
1:A:763:LEU:HD13	1:A:764:SER:H	0.57	1.60	2	1
1:B:855:LEU:HD13	1:B:856:LEU:N	0.57	2.13	2	2
1:C:775:LEU:O	1:C:775:LEU:HD22	0.57	1.99	14	2
1:B:667:ALA:CB	1:C:660:LEU:HD11	0.57	2.30	2	1
1:B:768:TYR:O	1:B:771:LEU:HD22	0.57	1.99	14	1
1:A:763:LEU:HD22	1:A:764:SER:H	0.57	1.60	7	2
1:A:821:ALA:O	1:A:822:VAL:HG13	0.57	2.00	5	1
1:B:829:VAL:O	1:B:833:VAL:HG22	0.57	1.99	7	2
1:C:695:LEU:HD22	1:C:695:LEU:O	0.57	2.00	10	1
1:B:764:SER:OG	1:B:771:LEU:HD12	0.57	1.99	12	2
1:B:816:ASN:ND2	1:B:830:ILE:HD12	0.57	2.13	8	1
1:A:686:ILE:HG12	1:B:686:ILE:HD12	0.57	1.75	8	2
1:C:702:LEU:C	1:C:702:LEU:HD13	0.57	2.19	10	7
1:A:781:ILE:HD13	1:B:746:ILE:HG12	0.57	1.74	3	2
1:A:819:ALA:HB1	1:A:826:THR:HB	0.57	1.76	7	5
1:A:790:TRP:CZ2	1:A:793:LEU:HD23	0.57	2.35	11	2
1:B:808:LYS:O	1:B:812:VAL:HG23	0.57	2.00	11	4
1:C:760:LEU:O	1:C:760:LEU:HD23	0.57	2.00	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:683:ARG:HG3	1:C:684:ILE:HD12	0.57	1.77	7	1
1:C:826:THR:O	1:C:830:ILE:HD12	0.57	1.99	8	1
1:A:750:ASN:CG	1:C:785:LEU:HD23	0.57	2.19	12	2
1:B:812:VAL:HG21	1:B:834:GLN:OE1	0.57	2.00	11	1
1:A:760:LEU:HD13	1:A:761:ARG:H	0.57	1.60	12	1
1:C:819:ALA:O	1:C:826:THR:HG21	0.56	2.00	7	2
1:B:693:ILE:HG12	1:C:692:LEU:HD21	0.56	1.77	14	1
1:A:754:ALA:HB2	1:B:715:LEU:HD11	0.56	1.77	4	1
1:A:771:LEU:C	1:A:771:LEU:HD13	0.56	2.20	7	1
1:C:774:LEU:O	1:C:778:VAL:HG23	0.56	2.00	13	1
1:A:715:LEU:HD12	1:C:751:GLY:O	0.56	1.99	6	1
1:C:828:ARG:O	1:C:832:VAL:HG12	0.56	2.00	11	2
1:B:793:LEU:HD11	1:B:847:ILE:CG1	0.56	2.30	12	1
1:A:753:LEU:HD23	1:C:791:GLU:HG3	0.56	1.76	14	1
1:B:765:LEU:HD23	1:B:774:LEU:HD11	0.56	1.77	15	1
1:B:763:LEU:H	1:B:763:LEU:HD13	0.56	1.61	5	4
1:C:764:SER:CB	1:C:771:LEU:HD12	0.56	2.30	13	1
1:C:830:ILE:HD13	1:C:830:ILE:O	0.56	2.01	7	4
1:A:808:LYS:O	1:A:812:VAL:HG22	0.56	2.01	2	4
1:A:714:PRO:HG3	1:C:705:VAL:HG22	0.56	1.76	1	2
1:B:761:ARG:O	1:B:765:LEU:HD22	0.56	2.01	7	1
1:A:785:LEU:HD23	1:B:750:ASN:CG	0.56	2.21	1	1
1:A:704:LEU:O	1:A:708:VAL:HG23	0.56	2.01	2	1
1:C:797:TRP:CG	1:C:847:ILE:HD12	0.56	2.36	3	3
1:B:821:ALA:O	1:B:822:VAL:HG13	0.56	2.01	4	1
1:C:660:LEU:C	1:C:661:LEU:HD23	0.56	2.21	4	1
1:A:781:ILE:HG23	1:B:746:ILE:CG2	0.56	2.31	13	1
1:B:751:GLY:HA2	1:C:715:LEU:HD11	0.56	1.77	2	1
1:C:771:LEU:HD23	1:C:772:ARG:CZ	0.56	2.31	2	1
1:C:663:LEU:C	1:C:663:LEU:HD22	0.56	2.22	15	2
1:A:760:LEU:HD11	1:C:799:LEU:HB2	0.56	1.76	6	1
1:A:781:ILE:HG23	1:B:746:ILE:HG23	0.56	1.77	7	2
1:A:830:ILE:O	1:A:830:ILE:HD13	0.56	2.00	8	1
1:C:819:ALA:CB	1:C:826:THR:HG21	0.56	2.23	14	1
1:A:771:LEU:HD22	1:A:771:LEU:N	0.55	2.16	4	7
1:A:819:ALA:HB1	1:A:826:THR:HG22	0.55	1.77	9	1
1:B:812:VAL:HG11	1:B:834:GLN:OE1	0.55	2.02	14	1
1:C:763:LEU:O	1:C:774:LEU:HD13	0.55	2.00	9	2
1:A:704:LEU:HD21	1:B:707:ARG:HA	0.55	1.78	8	1
1:A:819:ALA:HB3	1:A:827:ASP:OD1	0.55	2.01	11	1
1:A:771:LEU:HD22	1:A:772:ARG:H	0.55	1.62	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:756:ILE:HD13	1:C:795:TYR:CB	0.55	2.31	10	1
1:A:793:LEU:HD11	1:A:847:ILE:HG13	0.55	1.77	4	1
1:A:816:ASN:HB2	1:A:830:ILE:HD11	0.55	1.76	3	2
1:B:771:LEU:HD23	1:B:772:ARG:HD3	0.55	1.79	8	1
1:C:850:GLY:O	1:C:854:ILE:HG23	0.55	2.02	8	1
1:A:705:VAL:HG11	1:A:745:SER:HB2	0.55	1.79	12	1
1:B:793:LEU:HD12	1:B:793:LEU:O	0.55	2.01	14	1
1:B:754:ALA:HB3	1:C:715:LEU:O	0.55	2.01	15	1
1:A:795:TYR:CB	1:B:756:ILE:HG21	0.55	2.32	1	1
1:A:764:SER:HB3	1:A:771:LEU:HD12	0.55	1.78	14	3
1:B:819:ALA:O	1:B:826:THR:HG21	0.55	2.02	9	2
1:B:806:GLU:HG3	1:C:771:LEU:HD21	0.55	1.77	15	1
1:C:771:LEU:HD23	1:C:772:ARG:NE	0.55	2.16	2	1
1:C:809:ASN:O	1:C:812:VAL:HG22	0.55	2.02	8	1
1:C:771:LEU:O	1:C:774:LEU:HD23	0.55	2.01	10	1
1:A:693:ILE:HD12	1:A:693:ILE:O	0.55	2.02	15	1
1:A:774:LEU:HD13	1:A:777:ILE:HD11	0.54	1.79	8	1
1:A:692:LEU:HD12	1:A:693:ILE:N	0.54	2.17	13	1
1:C:790:TRP:CZ2	1:C:793:LEU:HD23	0.54	2.37	1	1
1:B:771:LEU:HD22	1:B:771:LEU:C	0.54	2.22	2	1
1:B:745:SER:O	1:B:748:LEU:HD23	0.54	2.02	8	1
1:B:781:ILE:HG21	1:C:746:ILE:HG21	0.54	1.78	2	3
1:A:795:TYR:CZ	1:A:796:TRP:NE1	0.54	2.76	2	7
1:C:793:LEU:HD23	1:C:847:ILE:HD11	0.54	1.78	7	1
1:C:695:LEU:O	1:C:698:VAL:HG12	0.54	2.03	13	1
1:C:675:ILE:HG22	1:C:679:LEU:HD12	0.54	1.79	4	1
1:A:693:ILE:HD11	1:B:696:ARG:HE	0.54	1.61	15	3
1:A:763:LEU:O	1:A:774:LEU:HD22	0.54	2.03	3	5
1:A:679:LEU:O	1:A:682:ILE:HG22	0.54	2.03	3	1
1:C:695:LEU:O	1:C:695:LEU:HD23	0.54	2.03	1	4
1:A:742:ARG:HH11	1:A:746:ILE:HD11	0.54	1.63	6	1
1:B:715:LEU:C	1:B:715:LEU:HD13	0.54	2.23	9	1
1:A:753:LEU:O	1:A:756:ILE:HD12	0.54	2.01	11	1
1:C:771:LEU:HD23	1:C:772:ARG:HD2	0.54	1.79	11	1
1:B:693:ILE:CG1	1:C:692:LEU:HD21	0.54	2.33	14	1
1:A:686:ILE:HD11	1:C:686:ILE:CG2	0.54	2.33	2	3
1:A:764:SER:OG	1:A:771:LEU:HD12	0.54	2.02	2	2
1:A:695:LEU:C	1:A:695:LEU:HD23	0.54	2.23	3	2
1:A:856:LEU:HD13	1:A:856:LEU:N	0.54	2.18	5	1
1:B:785:LEU:HD23	1:C:750:ASN:CG	0.54	2.23	15	2
1:C:827:ASP:HA	1:C:830:ILE:HD11	0.54	1.79	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:771:LEU:HD23	1:B:772:ARG:H	0.54	1.61	14	2
1:C:820:ILE:HD13	1:C:826:THR:HG22	0.54	1.79	14	1
1:A:760:LEU:C	1:A:760:LEU:HD13	0.54	2.23	10	5
1:B:682:ILE:HD12	1:B:683:ARG:H	0.54	1.61	11	2
1:B:799:LEU:O	1:B:803:TRP:CE3	0.54	2.61	4	3
1:A:695:LEU:HD23	1:A:695:LEU:O	0.54	2.03	2	7
1:C:702:LEU:O	1:C:702:LEU:HD13	0.54	2.03	4	1
1:C:793:LEU:HD13	1:C:794:LYS:N	0.54	2.18	10	1
1:A:845:ARG:O	1:A:847:ILE:HD13	0.54	2.03	1	1
1:C:771:LEU:HD22	1:C:771:LEU:N	0.54	2.17	11	8
1:A:802:TYR:CE1	1:B:760:LEU:HD11	0.54	2.38	7	1
1:C:819:ALA:HB1	1:C:826:THR:HG23	0.54	1.80	11	1
1:A:704:LEU:HD11	1:B:707:ARG:CG	0.53	2.33	6	2
1:C:753:LEU:C	1:C:753:LEU:HD22	0.53	2.23	6	4
1:B:686:ILE:CG2	1:C:686:ILE:HD11	0.53	2.32	2	2
1:B:695:LEU:HD23	1:B:695:LEU:O	0.53	2.04	2	2
1:B:796:TRP:NE1	1:C:756:ILE:HD11	0.53	2.18	2	1
1:A:669:LEU:HD23	1:A:676:THR:HG23	0.53	1.80	8	1
1:B:669:LEU:HD23	1:B:676:THR:HG23	0.53	1.79	12	4
1:C:768:TYR:CG	1:C:771:LEU:HD11	0.53	2.38	13	1
1:A:774:LEU:HD13	1:A:774:LEU:O	0.53	2.03	13	2
1:B:710:GLN:O	1:B:715:LEU:HD23	0.53	2.03	4	1
1:A:694:GLY:O	1:A:697:ILE:HG22	0.53	2.04	11	6
1:C:705:VAL:HG21	1:C:748:LEU:CD1	0.53	2.33	7	1
1:A:693:ILE:C	1:A:693:ILE:HD13	0.53	2.24	2	4
1:A:785:LEU:HD21	1:B:750:ASN:ND2	0.53	2.18	11	2
1:B:693:ILE:CD1	1:C:692:LEU:HD23	0.53	2.34	13	2
1:B:812:VAL:HG11	1:B:834:GLN:HE21	0.53	1.61	10	1
1:C:775:LEU:HD22	1:C:775:LEU:C	0.53	2.23	11	2
1:B:797:TRP:CD1	1:B:847:ILE:HD11	0.53	2.38	12	1
1:A:790:TRP:CH2	1:A:851:LEU:HD22	0.53	2.38	13	1
1:C:771:LEU:HD22	1:C:771:LEU:H	0.53	1.63	11	2
1:A:770:ARG:O	1:A:773:ASP:N	0.53	2.42	13	2
1:C:790:TRP:CH2	1:C:793:LEU:HD13	0.53	2.37	7	1
1:A:707:ARG:HA	1:C:704:LEU:HD13	0.53	1.81	10	2
1:A:820:ILE:O	1:A:822:VAL:HG22	0.53	2.03	14	1
1:A:763:LEU:O	1:A:774:LEU:HD13	0.53	2.04	6	1
1:A:693:ILE:HG22	1:C:693:ILE:HD13	0.53	1.80	11	1
1:A:704:LEU:O	1:A:708:VAL:HG22	0.53	2.03	14	1
1:C:756:ILE:HD13	1:C:756:ILE:C	0.53	2.24	15	1
1:B:675:ILE:HD11	1:B:679:LEU:HD12	0.53	1.78	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:715:LEU:O	1:B:716:SER:C	0.53	2.48	4	1
1:B:803:TRP:CZ2	1:C:760:LEU:HD22	0.53	2.39	4	1
1:A:760:LEU:HD21	1:C:803:TRP:CH2	0.53	2.38	5	1
1:C:771:LEU:HD22	1:C:772:ARG:H	0.53	1.61	10	1
1:B:830:ILE:HD12	1:B:831:GLU:N	0.53	2.18	11	1
1:C:663:LEU:HD23	1:C:663:LEU:O	0.53	2.03	11	1
1:C:807:LEU:O	1:C:807:LEU:HD13	0.53	2.03	12	2
1:A:803:TRP:N	1:A:803:TRP:CE3	0.53	2.77	4	13
1:C:820:ILE:HD11	1:C:827:ASP:HB2	0.53	1.78	1	1
1:A:689:VAL:O	1:A:692:LEU:HD22	0.53	2.04	8	1
1:B:675:ILE:HD12	1:B:675:ILE:O	0.53	2.04	7	2
1:B:819:ALA:HB1	1:B:826:THR:CG2	0.53	2.34	15	2
1:B:697:ILE:HD11	1:C:696:ARG:HD2	0.53	1.81	7	1
1:B:753:LEU:HD22	1:B:753:LEU:O	0.53	2.04	7	3
1:A:675:ILE:HD12	1:A:678:TRP:CE3	0.52	2.38	1	2
1:B:803:TRP:N	1:B:803:TRP:CE3	0.52	2.77	15	11
1:C:836:ALA:O	1:C:840:ILE:HG23	0.52	2.04	8	2
1:B:743:ASP:HA	1:B:746:ILE:HD12	0.52	1.80	7	1
1:A:675:ILE:CD1	1:A:679:LEU:HD23	0.52	2.34	8	1
1:A:748:LEU:HD23	1:A:748:LEU:O	0.52	2.04	11	2
1:A:710:GLN:CG	1:A:715:LEU:HD22	0.52	2.34	9	1
1:A:763:LEU:HD22	1:A:763:LEU:C	0.52	2.24	2	1
1:A:663:LEU:HD22	1:A:663:LEU:C	0.52	2.25	6	4
1:B:667:ALA:CA	1:C:660:LEU:HD11	0.52	2.34	2	1
1:A:754:ALA:HB3	1:B:715:LEU:HD21	0.52	1.81	9	1
1:A:820:ILE:HD12	1:A:827:ASP:OD1	0.52	2.04	10	1
1:A:696:ARG:HD3	1:C:693:ILE:HD11	0.52	1.82	15	1
1:A:771:LEU:HD11	1:A:772:ARG:NH2	0.52	2.19	3	1
1:A:763:LEU:HD13	1:A:763:LEU:N	0.52	2.20	4	1
1:B:816:ASN:O	1:B:820:ILE:HD12	0.52	2.05	4	1
1:A:693:ILE:HD13	1:B:696:ARG:HE	0.52	1.64	8	1
1:A:747:ARG:HG3	1:C:785:LEU:HD21	0.52	1.81	12	1
1:B:806:GLU:CB	1:C:771:LEU:HD21	0.52	2.34	10	1
1:A:791:GLU:O	1:A:794:LYS:HD2	0.52	2.05	1	1
1:B:771:LEU:N	1:B:771:LEU:HD22	0.52	2.20	8	6
1:C:779:THR:O	1:C:782:VAL:HG12	0.52	2.04	3	1
1:A:707:ARG:HB3	1:C:704:LEU:HD11	0.52	1.81	4	1
1:B:771:LEU:N	1:B:771:LEU:HD13	0.52	2.19	6	1
1:B:781:ILE:HD13	1:C:746:ILE:HG23	0.52	1.82	6	1
1:B:822:VAL:CG1	1:B:826:THR:HG22	0.52	2.34	8	1
1:B:686:ILE:CG2	1:C:686:ILE:HD12	0.52	2.35	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:756:ILE:HG21	1:C:795:TYR:CB	0.52	2.34	1	2
1:C:675:ILE:HG23	1:C:678:TRP:CZ2	0.52	2.40	4	1
1:B:771:LEU:HD13	1:B:771:LEU:N	0.52	2.19	7	3
1:C:803:TRP:N	1:C:803:TRP:CE3	0.52	2.78	3	15
1:B:781:ILE:HD12	1:C:746:ILE:HG21	0.52	1.79	3	1
1:B:781:ILE:HD12	1:C:746:ILE:CG2	0.52	2.35	3	1
1:C:745:SER:O	1:C:748:LEU:HD12	0.52	2.04	4	1
1:A:760:LEU:HD22	1:A:760:LEU:O	0.52	2.03	13	5
1:A:713:SER:O	1:A:714:PRO:C	0.52	2.49	11	5
1:C:794:LYS:HD3	1:C:795:TYR:N	0.52	2.19	6	1
1:C:678:TRP:CD1	1:C:682:ILE:HG21	0.52	2.40	11	1
1:A:697:ILE:HD13	1:A:698:VAL:H	0.52	1.65	4	3
1:A:795:TYR:CD1	1:B:756:ILE:HG23	0.52	2.40	11	1
1:A:803:TRP:N	1:A:803:TRP:HE3	0.51	2.04	1	7
1:C:753:LEU:HD12	1:C:754:ALA:N	0.51	2.19	1	1
1:B:819:ALA:HB3	1:B:830:ILE:HD11	0.51	1.82	15	1
1:B:667:ALA:HB2	1:C:660:LEU:CD1	0.51	2.35	2	1
1:A:836:ALA:O	1:A:840:ILE:HG23	0.51	2.06	9	2
1:C:695:LEU:HD13	1:C:696:ARG:HD2	0.51	1.81	10	1
1:C:826:THR:O	1:C:830:ILE:HG22	0.51	2.05	12	1
1:C:777:ILE:O	1:C:781:ILE:HG22	0.51	2.05	15	1
1:B:803:TRP:N	1:B:803:TRP:HE3	0.51	2.03	13	5
1:A:808:LYS:O	1:A:812:VAL:HG23	0.51	2.05	15	4
1:B:795:TYR:O	1:B:799:LEU:HD12	0.51	2.04	13	1
1:B:704:LEU:HD22	1:C:710:GLN:HG3	0.51	1.83	1	1
1:B:814:LEU:O	1:B:818:THR:HG22	0.51	2.05	1	1
1:A:760:LEU:HA	1:A:763:LEU:HD22	0.51	1.81	5	1
1:B:828:ARG:O	1:B:832:VAL:HG22	0.51	2.05	7	3
1:C:819:ALA:CB	1:C:830:ILE:HD11	0.51	2.34	8	1
1:A:756:ILE:HG21	1:C:795:TYR:CD2	0.51	2.41	12	1
1:A:791:GLU:HG3	1:B:753:LEU:HD13	0.51	1.82	1	1
1:A:763:LEU:HD13	1:A:764:SER:N	0.51	2.21	2	1
1:C:785:LEU:HD23	1:C:788:ARG:HD3	0.51	1.83	3	1
1:A:754:ALA:HB1	1:B:715:LEU:CB	0.51	2.35	7	1
1:A:826:THR:O	1:A:830:ILE:HG22	0.51	2.06	1	1
1:C:781:ILE:HG22	1:C:785:LEU:HD11	0.51	1.83	3	1
1:C:840:ILE:HD13	1:C:840:ILE:O	0.51	2.05	3	2
1:C:702:LEU:HD13	1:C:703:SER:N	0.51	2.20	5	3
1:A:793:LEU:HD13	1:A:847:ILE:HD12	0.51	1.83	6	1
1:A:816:ASN:CG	1:A:830:ILE:HD11	0.51	2.26	7	1
1:B:763:LEU:HD22	1:B:763:LEU:C	0.51	2.26	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:819:ALA:HB3	1:B:827:ASP:HB3	0.51	1.83	1	1
1:B:799:LEU:CD2	1:C:756:ILE:HD12	0.51	2.36	8	1
1:A:693:ILE:HD12	1:B:692:LEU:HD23	0.51	1.82	7	1
1:A:692:LEU:H	1:A:692:LEU:HD13	0.51	1.66	8	1
1:A:806:GLU:HB3	1:B:771:LEU:HD21	0.51	1.83	11	2
1:C:748:LEU:HD22	1:C:748:LEU:C	0.51	2.27	8	1
1:A:826:THR:O	1:A:829:VAL:HG12	0.51	2.06	10	1
1:A:796:TRP:HA	1:A:799:LEU:HD22	0.51	1.82	11	1
1:A:693:ILE:HD13	1:B:696:ARG:NE	0.50	2.20	8	1
1:C:793:LEU:HD13	1:C:793:LEU:C	0.50	2.26	10	1
1:C:843:ILE:H	1:C:843:ILE:HD13	0.50	1.65	7	1
1:A:750:ASN:O	1:A:753:LEU:HD23	0.50	2.07	10	1
1:A:756:ILE:H	1:A:756:ILE:HD12	0.50	1.65	2	1
1:A:771:LEU:HD23	1:A:771:LEU:H	0.50	1.65	13	1
1:C:759:ASP:O	1:C:763:LEU:HD22	0.50	2.05	13	1
1:A:828:ARG:O	1:A:832:VAL:HG12	0.50	2.07	3	5
1:A:760:LEU:HD11	1:C:803:TRP:CZ2	0.50	2.42	3	1
1:B:697:ILE:HD11	1:C:696:ARG:HB3	0.50	1.83	3	1
1:C:797:TRP:CD1	1:C:847:ILE:HD12	0.50	2.42	4	3
1:A:785:LEU:HD13	1:B:749:VAL:CB	0.50	2.36	5	1
1:C:778:VAL:O	1:C:781:ILE:HG22	0.50	2.07	12	1
1:A:754:ALA:HB3	1:B:715:LEU:HD22	0.50	1.81	14	2
1:B:675:ILE:HD12	1:B:678:TRP:CZ3	0.50	2.41	2	1
1:A:781:ILE:CG2	1:B:746:ILE:HG23	0.50	2.32	4	1
1:B:704:LEU:HD13	1:C:707:ARG:HA	0.50	1.82	4	1
1:A:669:LEU:HD23	1:A:670:TRP:CZ3	0.50	2.41	5	1
1:A:753:LEU:C	1:A:753:LEU:HD12	0.50	2.27	7	3
1:B:778:VAL:HA	1:B:781:ILE:HD11	0.50	1.83	1	1
1:A:760:LEU:HD21	1:C:803:TRP:CZ2	0.50	2.42	5	2
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.50	1.83	6	1
1:B:663:LEU:HD13	1:B:663:LEU:O	0.50	2.07	7	1
1:C:774:LEU:HD22	1:C:774:LEU:C	0.50	2.27	12	1
1:A:816:ASN:O	1:A:820:ILE:HD13	0.50	2.07	3	1
1:C:796:TRP:HA	1:C:799:LEU:HD22	0.50	1.84	3	1
1:A:746:ILE:HG12	1:C:781:ILE:HD13	0.50	1.84	4	1
1:C:790:TRP:CZ3	1:C:792:ALA:HB3	0.50	2.42	7	1
1:A:682:ILE:C	1:A:682:ILE:HD13	0.50	2.27	9	1
1:B:751:GLY:O	1:C:715:LEU:HD21	0.50	2.06	9	1
1:A:742:ARG:CZ	1:C:765:LEU:HD11	0.50	2.36	11	1
1:C:698:VAL:HG23	1:C:699:PHE:HD2	0.50	1.66	12	1
1:A:764:SER:CB	1:A:771:LEU:HD12	0.50	2.37	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:799:LEU:HD13	1:B:756:ILE:HD12	0.49	1.84	3	1
1:C:835:GLY:O	1:C:839:ALA:HB3	0.49	2.07	5	1
1:B:672:TRP:HB3	1:B:675:ILE:HG23	0.49	1.83	14	1
1:A:697:ILE:HD13	1:A:698:VAL:N	0.49	2.22	3	3
1:B:775:LEU:H	1:B:775:LEU:HD22	0.49	1.66	6	1
1:C:742:ARG:O	1:C:746:ILE:HD13	0.49	2.06	6	2
1:A:759:ASP:O	1:A:763:LEU:HD22	0.49	2.07	8	1
1:B:748:LEU:HD23	1:C:714:PRO:CB	0.49	2.37	10	1
1:A:750:ASN:ND2	1:C:781:ILE:HD11	0.49	2.22	11	1
1:B:826:THR:O	1:B:829:VAL:HG22	0.49	2.08	15	1
1:A:795:TYR:CE1	1:A:796:TRP:CD1	0.49	3.01	7	5
1:A:703:SER:OG	1:C:700:ALA:HB1	0.49	2.07	6	1
1:C:847:ILE:HD12	1:C:848:ARG:N	0.49	2.23	7	1
1:C:697:ILE:HD12	1:C:698:VAL:N	0.49	2.22	8	1
1:A:793:LEU:HD13	1:A:847:ILE:CG1	0.49	2.38	2	1
1:B:686:ILE:HG23	1:C:686:ILE:CD1	0.49	2.37	3	1
1:B:715:LEU:C	1:B:715:LEU:HD22	0.49	2.27	15	1
1:A:756:ILE:HD12	1:A:756:ILE:N	0.49	2.23	6	3
1:C:856:LEU:HD22	1:C:856:LEU:C	0.49	2.28	7	1
1:A:708:VAL:HG12	1:A:741:ASP:CG	0.49	2.28	8	1
1:B:843:ILE:H	1:B:843:ILE:HD13	0.49	1.66	12	1
1:B:695:LEU:HD21	1:B:699:PHE:CE2	0.49	2.42	1	1
1:C:685:PHE:O	1:C:689:VAL:HG23	0.49	2.07	2	2
1:A:708:VAL:HG11	1:B:713:SER:HA	0.49	1.83	3	1
1:A:791:GLU:HB3	1:B:753:LEU:HD23	0.49	1.85	7	2
1:A:793:LEU:CD1	1:A:847:ILE:HD11	0.49	2.38	7	1
1:B:694:GLY:HA2	1:B:697:ILE:HD13	0.49	1.84	7	1
1:C:793:LEU:HD12	1:C:848:ARG:CB	0.49	2.38	10	1
1:C:715:LEU:HD22	1:C:715:LEU:C	0.49	2.27	2	1
1:C:748:LEU:C	1:C:748:LEU:HD22	0.49	2.28	4	1
1:A:799:LEU:O	1:A:803:TRP:CD2	0.49	2.66	13	2
1:A:830:ILE:HD13	1:A:831:GLU:H	0.49	1.67	7	1
1:B:797:TRP:CD2	1:B:847:ILE:HD11	0.49	2.43	12	1
1:A:854:ILE:H	1:A:854:ILE:HD13	0.49	1.67	2	1
1:C:828:ARG:O	1:C:832:VAL:HG22	0.49	2.08	4	4
1:A:785:LEU:C	1:A:785:LEU:HD13	0.49	2.28	12	1
1:A:830:ILE:HD12	1:A:830:ILE:O	0.49	2.07	15	1
1:A:757:TRP:CH2	1:B:715:LEU:HD13	0.49	2.43	4	1
1:C:799:LEU:HD23	1:C:800:LEU:HG	0.49	1.84	4	1
1:A:756:ILE:O	1:A:760:LEU:HB3	0.49	2.06	15	4
1:A:785:LEU:HD11	1:B:746:ILE:HG23	0.49	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:819:ALA:HB1	1:C:826:THR:HB	0.49	1.85	13	4
1:A:792:ALA:HA	1:A:795:TYR:CE2	0.49	2.42	6	1
1:B:760:LEU:HD12	1:B:760:LEU:C	0.49	2.27	8	1
1:C:750:ASN:N	1:C:750:ASN:HD22	0.49	2.06	14	1
1:A:693:ILE:HD11	1:B:696:ARG:CD	0.48	2.38	1	1
1:B:843:ILE:O	1:B:843:ILE:HG23	0.48	2.08	1	5
1:B:820:ILE:O	1:B:822:VAL:N	0.48	2.46	4	1
1:B:781:ILE:HD13	1:C:746:ILE:CG2	0.48	2.38	6	1
1:A:785:LEU:HD13	1:A:785:LEU:C	0.48	2.29	14	1
1:A:702:LEU:C	1:A:702:LEU:HD13	0.48	2.28	15	1
1:C:672:TRP:O	1:C:674:ASP:N	0.48	2.46	15	1
1:A:695:LEU:HD22	1:A:696:ARG:NH1	0.48	2.23	3	1
1:C:803:TRP:N	1:C:803:TRP:HE3	0.48	2.07	7	3
1:B:764:SER:HB2	1:B:771:LEU:HD12	0.48	1.84	10	1
1:B:830:ILE:HD13	1:B:830:ILE:O	0.48	2.08	8	1
1:B:815:LEU:CD2	1:B:830:ILE:HD13	0.48	2.38	11	1
1:B:836:ALA:O	1:B:840:ILE:HD13	0.48	2.09	11	1
1:B:843:ILE:HD13	1:B:843:ILE:N	0.48	2.23	12	1
1:C:830:ILE:HG22	1:C:834:GLN:NE2	0.48	2.22	13	1
1:C:799:LEU:HD23	1:C:800:LEU:H	0.48	1.68	3	1
1:A:820:ILE:HD11	1:A:827:ASP:HB3	0.48	1.84	6	1
1:C:683:ARG:O	1:C:687:ILE:HD12	0.48	2.08	10	1
1:B:771:LEU:HD23	1:B:771:LEU:N	0.48	2.23	15	2
1:B:791:GLU:OE2	1:C:753:LEU:HD13	0.48	2.08	15	1
1:B:763:LEU:C	1:B:763:LEU:HD22	0.48	2.29	4	1
1:A:704:LEU:HD12	1:B:712:TYR:O	0.48	2.08	5	1
1:A:795:TYR:CD2	1:B:753:LEU:HA	0.48	2.43	6	1
1:B:803:TRP:CH2	1:C:768:TYR:CZ	0.48	3.02	7	1
1:B:672:TRP:N	1:B:672:TRP:CD1	0.48	2.81	8	2
1:C:760:LEU:C	1:C:760:LEU:HD13	0.48	2.29	15	1
1:C:694:GLY:O	1:C:697:ILE:HG22	0.48	2.08	2	1
1:A:768:TYR:C	1:A:770:ARG:H	0.48	2.11	13	3
1:A:675:ILE:HD11	1:A:678:TRP:CE3	0.48	2.44	12	1
1:A:820:ILE:HD11	1:A:827:ASP:OD2	0.48	2.09	14	1
1:B:779:THR:O	1:B:782:VAL:HG12	0.48	2.09	1	1
1:B:742:ARG:O	1:B:746:ILE:HD12	0.48	2.09	5	1
1:A:771:LEU:HD12	1:A:772:ARG:CZ	0.48	2.38	7	1
1:A:771:LEU:HD23	1:A:771:LEU:N	0.48	2.23	13	1
1:A:760:LEU:CD2	1:A:763:LEU:HD21	0.48	2.38	14	1
1:B:685:PHE:HA	1:B:688:ILE:HD12	0.48	1.85	2	1
1:C:828:ARG:O	1:C:832:VAL:HG13	0.48	2.09	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:660:LEU:HD12	1:C:661:LEU:H	0.48	1.69	14	1
1:A:771:LEU:HD22	1:A:771:LEU:H	0.48	1.69	4	2
1:C:781:ILE:O	1:C:781:ILE:HD13	0.48	2.08	9	1
1:B:715:LEU:HD12	1:B:715:LEU:C	0.48	2.29	4	1
1:B:753:LEU:HD22	1:B:753:LEU:C	0.48	2.28	6	2
1:B:771:LEU:HD23	1:B:772:ARG:HD2	0.48	1.85	10	1
1:A:753:LEU:HD22	1:A:753:LEU:O	0.47	2.09	1	2
1:A:750:ASN:HD21	1:C:785:LEU:HD23	0.47	1.69	15	2
1:A:843:ILE:N	1:A:843:ILE:HD12	0.47	2.24	3	1
1:A:696:ARG:HG3	1:C:693:ILE:HD11	0.47	1.86	12	2
1:C:816:ASN:O	1:C:820:ILE:HD13	0.47	2.09	4	1
1:B:768:TYR:HD1	1:B:771:LEU:HD11	0.47	1.69	10	1
1:C:763:LEU:HD22	1:C:763:LEU:C	0.47	2.28	10	1
1:A:791:GLU:CB	1:B:753:LEU:HD22	0.47	2.39	12	1
1:B:697:ILE:HD11	1:C:699:PHE:CE1	0.47	2.44	1	1
1:C:830:ILE:HD13	1:C:830:ILE:C	0.47	2.30	7	2
1:B:686:ILE:HG23	1:C:686:ILE:HD11	0.47	1.84	3	1
1:A:785:LEU:HD13	1:B:749:VAL:CG2	0.47	2.38	5	1
1:A:692:LEU:HD23	1:C:693:ILE:CD1	0.47	2.38	6	1
1:A:799:LEU:HD13	1:B:756:ILE:HG22	0.47	1.84	9	1
1:B:785:LEU:HD21	1:C:747:ARG:NH1	0.47	2.24	15	1
1:B:803:TRP:CE3	1:B:803:TRP:N	0.47	2.83	4	3
1:B:742:ARG:O	1:B:746:ILE:HD13	0.47	2.09	3	1
1:B:808:LYS:O	1:B:812:VAL:HG12	0.47	2.09	14	3
1:A:792:ALA:O	1:A:795:TYR:CD2	0.47	2.67	14	4
1:B:669:LEU:C	1:B:669:LEU:HD12	0.47	2.30	8	1
1:B:797:TRP:CE2	1:B:847:ILE:HD11	0.47	2.44	10	1
1:B:815:LEU:HD21	1:B:830:ILE:HD13	0.47	1.85	11	1
1:B:820:ILE:HD11	1:B:827:ASP:HB2	0.47	1.86	11	1
1:A:774:LEU:HD21	1:B:742:ARG:NH2	0.47	2.24	13	1
1:B:705:VAL:HG12	1:B:709:ARG:NH2	0.47	2.24	13	1
1:A:796:TRP:NE1	1:B:756:ILE:HD13	0.47	2.23	1	1
1:A:851:LEU:HD13	1:A:851:LEU:O	0.47	2.08	4	1
1:B:806:GLU:OE2	1:C:771:LEU:HD21	0.47	2.09	4	1
1:A:793:LEU:HD12	1:A:797:TRP:HE1	0.47	1.67	11	1
1:B:675:ILE:HD12	1:B:678:TRP:CE3	0.47	2.45	2	2
1:B:855:LEU:HD23	1:B:855:LEU:O	0.47	2.09	1	1
1:A:663:LEU:HD13	1:A:663:LEU:C	0.47	2.29	14	2
1:B:771:LEU:HD13	1:B:771:LEU:H	0.47	1.68	6	1
1:C:799:LEU:O	1:C:803:TRP:CE3	0.47	2.68	7	1
1:B:854:ILE:O	1:B:854:ILE:HG22	0.47	2.09	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:793:LEU:HD12	1:B:797:TRP:NE1	0.47	2.25	3	1
1:C:808:LYS:O	1:C:812:VAL:HG23	0.47	2.09	4	5
1:B:768:TYR:CD1	1:B:771:LEU:HD11	0.47	2.43	10	1
1:A:774:LEU:HD13	1:A:774:LEU:C	0.47	2.30	4	3
1:B:785:LEU:HD21	1:C:750:ASN:ND2	0.47	2.24	2	1
1:A:742:ARG:O	1:A:746:ILE:HD12	0.47	2.10	6	1
1:B:700:ALA:HB1	1:C:703:SER:OG	0.47	2.10	10	1
1:C:775:LEU:HD22	1:C:775:LEU:O	0.47	2.09	11	1
1:A:705:VAL:HG11	1:A:745:SER:CB	0.47	2.39	12	1
1:A:847:ILE:HG23	1:A:848:ARG:N	0.47	2.25	12	1
1:C:663:LEU:HD13	1:C:663:LEU:H	0.47	1.69	12	1
1:B:660:LEU:N	1:B:660:LEU:HD12	0.47	2.25	13	1
1:A:753:LEU:HA	1:C:791:GLU:OE2	0.47	2.09	14	1
1:A:770:ARG:O	1:A:774:LEU:N	0.47	2.48	11	5
1:A:715:LEU:HD12	1:C:751:GLY:HA3	0.47	1.87	2	1
1:B:687:ILE:HD12	1:B:687:ILE:H	0.47	1.69	2	1
1:B:754:ALA:HB1	1:C:715:LEU:HB3	0.47	1.87	3	1
1:C:808:LYS:O	1:C:812:VAL:HG12	0.47	2.09	11	2
1:A:760:LEU:HD22	1:A:760:LEU:C	0.47	2.30	13	1
1:A:753:LEU:HD13	1:A:753:LEU:C	0.47	2.30	15	1
1:A:765:LEU:HD12	1:A:770:ARG:HH21	0.47	1.68	1	1
1:C:829:VAL:O	1:C:833:VAL:HG12	0.47	2.09	1	1
1:A:781:ILE:HG21	1:B:746:ILE:HG21	0.47	1.87	8	2
1:B:710:GLN:CD	1:B:715:LEU:HD21	0.47	2.30	3	1
1:A:746:ILE:CG2	1:C:781:ILE:HG21	0.47	2.40	5	3
1:A:750:ASN:HD21	1:C:785:LEU:HD13	0.47	1.69	6	1
1:B:705:VAL:CG2	1:B:748:LEU:HD13	0.47	2.40	6	1
1:C:793:LEU:HD12	1:C:848:ARG:HB2	0.47	1.87	10	1
1:A:836:ALA:O	1:A:840:ILE:HD13	0.47	2.09	11	1
1:B:794:LYS:HD3	1:B:795:TYR:N	0.47	2.25	2	5
1:C:790:TRP:C	1:C:792:ALA:N	0.47	2.68	5	5
1:A:791:GLU:O	1:A:795:TYR:CD2	0.47	2.68	6	1
1:C:750:ASN:O	1:C:753:LEU:HD12	0.47	2.10	7	1
1:A:663:LEU:HD13	1:B:660:LEU:CB	0.47	2.40	8	1
1:A:707:ARG:NH2	1:A:712:TYR:CZ	0.47	2.83	11	1
1:A:669:LEU:HD12	1:A:676:THR:HG23	0.46	1.86	1	1
1:B:793:LEU:C	1:B:793:LEU:HD13	0.46	2.30	12	2
1:C:847:ILE:H	1:C:847:ILE:HD13	0.46	1.69	9	2
1:B:847:ILE:C	1:B:847:ILE:HD13	0.46	2.30	15	1
1:B:796:TRP:CD1	1:C:756:ILE:HD11	0.46	2.45	3	1
1:C:832:VAL:O	1:C:836:ALA:HB2	0.46	2.10	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:820:ILE:HD12	1:A:820:ILE:N	0.46	2.25	12	3
1:A:755:LEU:HD22	1:A:755:LEU:C	0.46	2.30	8	1
1:A:790:TRP:CE2	1:A:793:LEU:HD23	0.46	2.45	15	2
1:A:707:ARG:HB3	1:C:704:LEU:HD21	0.46	1.86	12	2
1:A:802:TYR:CD1	1:B:768:TYR:CZ	0.46	3.03	14	1
1:B:799:LEU:HD13	1:C:756:ILE:HG23	0.46	1.87	2	1
1:C:687:ILE:H	1:C:687:ILE:HD12	0.46	1.70	13	1
1:A:771:LEU:H	1:A:771:LEU:CD1	0.46	2.22	15	1
1:A:678:TRP:CD1	1:A:682:ILE:HD13	0.46	2.45	2	2
1:B:822:VAL:HG12	1:B:826:THR:CG2	0.46	2.38	8	1
1:B:760:LEU:HD22	1:B:760:LEU:C	0.46	2.30	12	4
1:B:679:LEU:HD13	1:B:679:LEU:O	0.46	2.10	5	1
1:A:692:LEU:HD23	1:C:693:ILE:HD11	0.46	1.87	6	1
1:B:828:ARG:O	1:B:832:VAL:HG13	0.46	2.11	10	3
1:B:684:ILE:HD12	1:B:684:ILE:N	0.46	2.25	8	3
1:C:826:THR:O	1:C:829:VAL:HG22	0.46	2.10	11	1
1:A:771:LEU:HD13	1:A:771:LEU:N	0.46	2.23	15	2
1:C:790:TRP:CE3	1:C:793:LEU:HD12	0.46	2.46	5	1
1:A:763:LEU:HB2	1:A:774:LEU:HD22	0.46	1.88	7	1
1:C:843:ILE:HD13	1:C:843:ILE:O	0.46	2.10	13	1
1:A:779:THR:O	1:A:782:VAL:HG12	0.46	2.10	2	1
1:C:856:LEU:HD22	1:C:856:LEU:O	0.46	2.11	7	1
1:A:819:ALA:HB3	1:A:827:ASP:CG	0.46	2.31	10	1
1:B:669:LEU:HD12	1:B:676:THR:HG23	0.46	1.86	1	1
1:A:847:ILE:HD13	1:A:847:ILE:H	0.46	1.70	3	1
1:C:764:SER:O	1:C:765:LEU:O	0.46	2.33	7	1
1:B:843:ILE:HD13	1:B:844:PRO:N	0.46	2.26	11	1
1:A:707:ARG:CG	1:C:704:LEU:HD11	0.46	2.40	1	1
1:A:790:TRP:C	1:A:792:ALA:N	0.46	2.67	2	13
1:C:663:LEU:HD13	1:C:664:ASP:H	0.46	1.71	2	1
1:A:693:ILE:HG13	1:B:693:ILE:HG22	0.46	1.88	5	1
1:A:700:ALA:HB1	1:B:703:SER:OG	0.46	2.11	6	1
1:A:753:LEU:HD22	1:C:788:ARG:O	0.46	2.10	8	1
1:C:705:VAL:HG22	1:C:748:LEU:HD11	0.46	1.87	9	1
1:C:822:VAL:HG22	1:C:823:GLY:N	0.46	2.26	12	1
1:A:843:ILE:O	1:A:843:ILE:HG23	0.46	2.11	14	1
1:B:774:LEU:O	1:B:777:ILE:HG13	0.46	2.11	14	1
1:C:819:ALA:HB3	1:C:826:THR:CG2	0.46	2.24	14	1
1:A:847:ILE:HD13	1:A:847:ILE:N	0.46	2.26	1	1
1:A:781:ILE:HG21	1:B:746:ILE:HG22	0.46	1.87	2	1
1:C:675:ILE:HD12	1:C:678:TRP:CE3	0.46	2.45	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:686:ILE:CD1	1:C:686:ILE:HG21	0.46	2.41	5	1
1:C:661:LEU:HD22	1:C:661:LEU:N	0.46	2.26	6	1
1:C:790:TRP:CH2	1:C:851:LEU:HD22	0.46	2.46	6	1
1:B:830:ILE:HD13	1:B:830:ILE:C	0.46	2.30	8	1
1:B:705:VAL:HG22	1:C:714:PRO:HG3	0.46	1.87	10	1
1:C:799:LEU:HD22	1:C:803:TRP:CE2	0.46	2.44	11	1
1:A:796:TRP:CD1	1:A:799:LEU:HD12	0.46	2.45	15	1
1:C:662:GLU:O	1:C:663:LEU:HD12	0.46	2.10	15	1
1:A:803:TRP:CE3	1:A:803:TRP:N	0.45	2.84	3	2
1:B:667:ALA:HB2	1:C:660:LEU:CD2	0.45	2.41	5	1
1:B:750:ASN:ND2	1:B:750:ASN:H	0.45	2.09	6	3
1:B:812:VAL:HG21	1:B:834:GLN:HG3	0.45	1.87	8	1
1:C:819:ALA:HB1	1:C:826:THR:CB	0.45	2.41	8	1
1:C:763:LEU:C	1:C:774:LEU:HD13	0.45	2.31	9	1
1:A:829:VAL:O	1:A:833:VAL:HG12	0.45	2.11	15	1
1:C:778:VAL:HA	1:C:781:ILE:HD12	0.45	1.87	4	1
1:A:693:ILE:O	1:A:693:ILE:HD13	0.45	2.12	5	2
1:B:775:LEU:HD13	1:B:776:LEU:N	0.45	2.26	11	1
1:B:711:GLY:O	1:B:713:SER:N	0.45	2.48	12	1
1:A:714:PRO:CG	1:C:705:VAL:HG22	0.45	2.41	1	2
1:C:713:SER:O	1:C:714:PRO:C	0.45	2.54	2	5
1:B:675:ILE:HD13	1:B:675:ILE:C	0.45	2.32	8	1
1:A:777:ILE:O	1:A:781:ILE:HD12	0.45	2.11	9	1
1:B:792:ALA:HA	1:B:795:TYR:CZ	0.45	2.47	11	1
1:C:822:VAL:HG13	1:C:823:GLY:H	0.45	1.71	12	1
1:A:702:LEU:HD13	1:A:706:ASN:OD1	0.45	2.12	1	1
1:B:771:LEU:HA	1:B:774:LEU:HD23	0.45	1.88	2	1
1:A:795:TYR:CZ	1:A:796:TRP:CD1	0.45	3.05	5	2
1:B:834:GLN:HG3	1:B:835:GLY:N	0.45	2.26	5	1
1:C:705:VAL:HG21	1:C:748:LEU:HD22	0.45	1.88	5	1
1:A:756:ILE:HG23	1:C:799:LEU:CD2	0.45	2.41	12	1
1:A:689:VAL:O	1:A:692:LEU:HD11	0.45	2.10	13	1
1:A:833:VAL:HG23	1:A:834:GLN:NE2	0.45	2.27	6	1
1:C:785:LEU:HD12	1:C:786:GLY:N	0.45	2.27	6	1
1:B:697:ILE:HD12	1:B:697:ILE:N	0.45	2.26	7	1
1:B:753:LEU:O	1:B:756:ILE:HG22	0.45	2.12	15	2
1:A:693:ILE:HG21	1:B:693:ILE:HG22	0.45	1.87	11	2
1:A:791:GLU:OE2	1:B:753:LEU:HD13	0.45	2.10	12	2
1:B:820:ILE:HD11	1:B:827:ASP:CB	0.45	2.41	11	1
1:A:683:ARG:O	1:A:687:ILE:HD12	0.45	2.11	13	1
1:B:678:TRP:CD1	1:B:678:TRP:C	0.45	2.90	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:816:ASN:HA	1:A:830:ILE:HG21	0.45	1.89	8	1
1:A:778:VAL:O	1:A:782:VAL:HG23	0.45	2.11	9	1
1:C:760:LEU:HD22	1:C:760:LEU:C	0.45	2.31	1	1
1:A:851:LEU:C	1:A:851:LEU:HD13	0.45	2.32	15	3
1:A:750:ASN:CG	1:C:785:LEU:HD21	0.45	2.32	4	1
1:A:744:ARG:O	1:A:747:ARG:HB2	0.45	2.12	9	1
1:B:791:GLU:HB3	1:C:753:LEU:HD23	0.45	1.89	9	1
1:B:762:SER:O	1:B:765:LEU:HD23	0.45	2.11	14	1
1:A:678:TRP:C	1:A:678:TRP:CD1	0.45	2.90	9	2
1:A:705:VAL:HG21	1:A:748:LEU:CD1	0.45	2.40	10	1
1:A:828:ARG:O	1:A:832:VAL:HG23	0.45	2.12	9	2
1:B:760:LEU:HD13	1:B:760:LEU:C	0.45	2.32	1	1
1:B:744:ARG:O	1:B:747:ARG:HB2	0.45	2.11	3	1
1:A:791:GLU:HG2	1:B:753:LEU:HD23	0.45	1.89	10	1
1:B:791:GLU:OE1	1:C:753:LEU:HD23	0.45	2.12	11	1
1:A:686:ILE:CG1	1:B:686:ILE:HD11	0.45	2.42	12	1
1:B:704:LEU:HD13	1:C:707:ARG:HB2	0.45	1.89	13	1
1:C:776:LEU:O	1:C:776:LEU:HD23	0.45	2.11	14	2
1:C:678:TRP:C	1:C:678:TRP:CD1	0.45	2.91	7	1
1:A:756:ILE:HG23	1:C:799:LEU:HD21	0.45	1.89	12	1
1:A:692:LEU:HD12	1:A:693:ILE:H	0.45	1.71	13	1
1:C:843:ILE:N	1:C:844:PRO:CD	0.45	2.80	13	2
1:B:753:LEU:HD13	1:B:753:LEU:C	0.44	2.32	7	2
1:A:819:ALA:O	1:A:822:VAL:HG22	0.44	2.12	11	1
1:B:771:LEU:HD22	1:B:771:LEU:H	0.44	1.72	1	1
1:B:663:LEU:C	1:B:663:LEU:HD13	0.44	2.33	2	1
1:C:695:LEU:C	1:C:695:LEU:HD23	0.44	2.32	6	1
1:A:777:ILE:HD12	1:A:778:VAL:N	0.44	2.28	8	1
1:B:771:LEU:HD23	1:B:772:ARG:CD	0.44	2.42	10	1
1:B:803:TRP:CE3	1:C:768:TYR:CZ	0.44	3.05	13	1
1:A:760:LEU:HD23	1:C:799:LEU:CD2	0.44	2.41	1	1
1:A:790:TRP:CE3	1:A:790:TRP:HA	0.44	2.47	5	2
1:B:855:LEU:HD13	1:B:855:LEU:C	0.44	2.33	2	1
1:C:829:VAL:O	1:C:833:VAL:HG23	0.44	2.12	4	2
1:A:663:LEU:HD11	1:B:660:LEU:HB2	0.44	1.88	5	1
1:A:750:ASN:ND2	1:C:785:LEU:HD13	0.44	2.26	6	1
1:A:771:LEU:C	1:A:771:LEU:CD1	0.44	2.86	7	1
1:A:795:TYR:CE2	1:A:796:TRP:CD1	0.44	3.06	14	2
1:B:704:LEU:HD13	1:B:704:LEU:O	0.44	2.13	9	1
1:C:771:LEU:HD13	1:C:771:LEU:N	0.44	2.26	10	1
1:B:704:LEU:HD21	1:C:707:ARG:HA	0.44	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:756:ILE:O	1:B:760:LEU:HB3	0.44	2.12	11	2
1:C:816:ASN:OD1	1:C:830:ILE:HG21	0.44	2.13	3	1
1:B:693:ILE:HD13	1:C:696:ARG:NE	0.44	2.26	12	1
1:A:669:LEU:HD22	1:A:669:LEU:N	0.44	2.27	3	1
1:C:763:LEU:HD23	1:C:763:LEU:C	0.44	2.33	3	2
1:A:795:TYR:HA	1:B:756:ILE:HD13	0.44	1.88	5	1
1:C:705:VAL:HG21	1:C:748:LEU:HD12	0.44	1.88	7	1
1:A:693:ILE:HD11	1:B:696:ARG:CZ	0.44	2.41	4	1
1:B:775:LEU:C	1:B:775:LEU:HD13	0.44	2.33	4	1
1:B:699:PHE:CD2	1:B:702:LEU:HD23	0.44	2.47	12	1
1:A:741:ASP:O	1:A:745:SER:N	0.44	2.50	3	2
1:A:755:LEU:HD13	1:A:755:LEU:C	0.44	2.32	8	1
1:B:816:ASN:OD1	1:B:830:ILE:HD11	0.44	2.12	1	1
1:B:790:TRP:C	1:B:792:ALA:N	0.44	2.71	14	7
1:B:713:SER:O	1:B:714:PRO:C	0.44	2.57	4	6
1:C:756:ILE:O	1:C:760:LEU:HG	0.44	2.13	4	1
1:B:763:LEU:O	1:B:774:LEU:CB	0.44	2.66	14	2
1:B:806:GLU:HG3	1:C:771:LEU:HD11	0.44	1.90	5	1
1:C:765:LEU:HD12	1:C:765:LEU:C	0.44	2.32	7	1
1:C:682:ILE:HD13	1:C:683:ARG:H	0.44	1.71	8	1
1:A:747:ARG:NE	1:C:785:LEU:HD21	0.44	2.27	9	1
1:A:820:ILE:HD12	1:A:827:ASP:CG	0.44	2.32	10	1
1:C:793:LEU:O	1:C:797:TRP:CD1	0.44	2.71	12	1
1:B:819:ALA:CB	1:B:830:ILE:HD11	0.44	2.42	15	1
1:A:712:TYR:O	1:C:704:LEU:HD11	0.44	2.13	3	2
1:B:774:LEU:O	1:B:778:VAL:HG23	0.44	2.12	3	1
1:A:826:THR:O	1:A:830:ILE:HD12	0.44	2.12	5	1
1:B:771:LEU:H	1:B:771:LEU:HD22	0.44	1.73	10	2
1:C:822:VAL:HG12	1:C:822:VAL:O	0.44	2.12	10	1
1:A:771:LEU:O	1:A:774:LEU:HD23	0.44	2.13	12	1
1:B:756:ILE:C	1:B:756:ILE:HD13	0.44	2.33	13	1
1:A:753:LEU:C	1:A:753:LEU:CD2	0.43	2.85	6	2
1:C:673:PHE:O	1:C:674:ASP:CB	0.43	2.66	2	1
1:B:797:TRP:CD1	1:B:847:ILE:HG21	0.43	2.48	3	1
1:A:795:TYR:CD1	1:B:756:ILE:HD13	0.43	2.48	6	1
1:B:754:ALA:HB1	1:C:715:LEU:O	0.43	2.13	6	1
1:A:760:LEU:HD23	1:A:763:LEU:HD21	0.43	1.89	7	1
1:B:796:TRP:CD1	1:C:756:ILE:HD13	0.43	2.48	7	1
1:B:710:GLN:OE1	1:B:715:LEU:HD11	0.43	2.13	8	1
1:A:715:LEU:O	1:C:754:ALA:HB1	0.43	2.13	9	1
1:B:663:LEU:C	1:B:663:LEU:HD12	0.43	2.33	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:769:HIS:N	1:B:771:LEU:HD22	0.43	2.28	11	1
1:C:703:SER:O	1:C:706:ASN:ND2	0.43	2.52	11	1
1:B:803:TRP:CE2	1:C:768:TYR:OH	0.43	2.65	13	1
1:A:679:LEU:HD21	1:C:683:ARG:HH12	0.43	1.73	15	1
1:A:686:ILE:CG2	1:B:686:ILE:HD11	0.43	2.43	15	1
1:B:688:ILE:HD12	1:B:688:ILE:N	0.43	2.28	10	3
1:B:774:LEU:C	1:B:774:LEU:HD13	0.43	2.33	4	1
1:C:799:LEU:O	1:C:803:TRP:CE2	0.43	2.71	5	1
1:C:695:LEU:HD23	1:C:695:LEU:O	0.43	2.13	6	1
1:C:790:TRP:O	1:C:790:TRP:CD1	0.43	2.71	6	1
1:C:749:VAL:HG23	1:C:750:ASN:N	0.43	2.29	8	1
1:A:753:LEU:HA	1:C:791:GLU:CD	0.43	2.34	14	1
1:A:771:LEU:HD21	1:C:806:GLU:HG2	0.43	1.89	15	1
1:A:678:TRP:CD1	1:A:678:TRP:C	0.43	2.91	11	6
1:B:702:LEU:C	1:B:702:LEU:CD1	0.43	2.87	10	2
1:B:774:LEU:HD13	1:B:774:LEU:O	0.43	2.13	10	1
1:B:855:LEU:C	1:B:855:LEU:HD12	0.43	2.33	11	1
1:C:822:VAL:HG22	1:C:822:VAL:O	0.43	2.12	11	1
1:B:768:TYR:O	1:B:771:LEU:CD1	0.43	2.66	12	1
1:A:663:LEU:O	1:A:663:LEU:HD23	0.43	2.14	15	1
1:A:830:ILE:HG23	1:A:831:GLU:N	0.43	2.29	1	1
1:A:693:ILE:HD13	1:A:693:ILE:C	0.43	2.34	3	1
1:B:707:ARG:NH1	1:C:712:TYR:O	0.43	2.52	7	1
1:B:847:ILE:HD11	1:B:851:LEU:CD1	0.43	2.44	7	1
1:B:768:TYR:O	1:B:769:HIS:CG	0.43	2.71	8	1
1:B:836:ALA:O	1:B:840:ILE:HD12	0.43	2.13	8	2
1:C:778:VAL:O	1:C:782:VAL:HG23	0.43	2.13	15	1
1:A:747:ARG:O	1:A:750:ASN:N	0.43	2.52	4	2
1:B:785:LEU:HD23	1:C:750:ASN:CB	0.43	2.43	10	1
1:C:742:ARG:O	1:C:746:ILE:HD12	0.43	2.14	12	1
1:C:851:LEU:O	1:C:851:LEU:HD13	0.43	2.14	12	1
1:B:771:LEU:HD23	1:B:771:LEU:H	0.43	1.73	13	1
1:A:704:LEU:N	1:A:704:LEU:HD22	0.43	2.28	14	1
1:A:756:ILE:O	1:A:760:LEU:CD1	0.43	2.67	4	1
1:B:803:TRP:HH2	1:C:760:LEU:HD22	0.43	1.69	4	1
1:C:702:LEU:HD13	1:C:702:LEU:C	0.43	2.33	4	2
1:B:812:VAL:HG12	1:B:816:ASN:OD1	0.43	2.13	8	1
1:B:748:LEU:C	1:B:748:LEU:HD12	0.43	2.34	9	1
1:C:851:LEU:HD13	1:C:851:LEU:C	0.43	2.34	12	1
1:A:771:LEU:HD21	1:C:806:GLU:HB2	0.43	1.90	14	1
1:B:760:LEU:C	1:B:760:LEU:HD23	0.43	2.34	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:775:LEU:C	1:C:775:LEU:HD13	0.43	2.34	15	1
1:C:797:TRP:HE1	1:C:847:ILE:HD13	0.43	1.74	2	1
1:A:747:ARG:O	1:A:750:ASN:HB2	0.43	2.12	4	1
1:A:822:VAL:CG2	1:A:826:THR:HG21	0.43	2.44	5	1
1:B:763:LEU:HD22	1:B:764:SER:H	0.43	1.73	7	1
1:A:832:VAL:HG23	1:A:833:VAL:N	0.43	2.28	11	2
1:A:847:ILE:HD12	1:A:848:ARG:N	0.43	2.28	11	2
1:B:750:ASN:HD22	1:B:750:ASN:N	0.43	2.12	11	1
1:B:669:LEU:HD22	1:B:679:LEU:HD22	0.43	1.90	13	1
1:B:812:VAL:HG22	1:B:816:ASN:OD1	0.43	2.14	14	1
1:C:660:LEU:HD12	1:C:661:LEU:N	0.43	2.29	14	1
1:B:704:LEU:HD11	1:C:707:ARG:HB3	0.43	1.89	2	1
1:C:689:VAL:O	1:C:693:ILE:HG23	0.43	2.14	3	1
1:C:763:LEU:HD23	1:C:764:SER:N	0.43	2.29	13	3
1:B:850:GLY:O	1:B:854:ILE:HD12	0.43	2.14	4	1
1:B:799:LEU:HD12	1:C:756:ILE:HD12	0.43	1.91	6	1
1:B:662:GLU:O	1:B:663:LEU:CB	0.43	2.67	7	1
1:A:795:TYR:HB2	1:B:756:ILE:HB	0.43	1.91	8	1
1:B:797:TRP:HE1	1:B:847:ILE:HG21	0.43	1.74	9	1
1:A:795:TYR:OH	1:B:755:LEU:HD23	0.43	2.13	11	1
1:A:704:LEU:HD11	1:B:707:ARG:HG2	0.43	1.90	12	1
1:C:748:LEU:C	1:C:748:LEU:HD13	0.43	2.34	12	1
1:B:803:TRP:CZ3	1:C:768:TYR:CE1	0.43	3.06	15	1
1:C:799:LEU:O	1:C:803:TRP:CD2	0.43	2.71	8	2
1:B:774:LEU:O	1:B:777:ILE:HD12	0.43	2.14	11	1
1:B:843:ILE:HD13	1:B:843:ILE:C	0.43	2.34	11	1
1:A:776:LEU:HD12	1:A:777:ILE:N	0.43	2.29	13	1
1:A:696:ARG:NE	1:C:693:ILE:HD11	0.43	2.29	1	1
1:A:790:TRP:CD1	1:A:793:LEU:HD23	0.43	2.49	2	1
1:A:781:ILE:O	1:A:785:LEU:HG	0.43	2.14	5	1
1:B:747:ARG:HA	1:B:750:ASN:HD21	0.43	1.74	6	1
1:A:715:LEU:HD12	1:A:715:LEU:N	0.43	2.29	11	1
1:A:776:LEU:O	1:A:779:THR:HG22	0.43	2.14	11	1
1:A:795:TYR:CZ	1:A:796:TRP:CE2	0.43	3.07	14	1
1:B:833:VAL:HG23	1:B:834:GLN:N	0.43	2.29	15	1
1:A:663:LEU:C	1:A:663:LEU:HD23	0.42	2.35	13	2
1:A:830:ILE:C	1:A:830:ILE:HD12	0.42	2.34	10	2
1:C:797:TRP:CB	1:C:847:ILE:HD12	0.42	2.44	3	1
1:A:763:LEU:HD23	1:A:763:LEU:C	0.42	2.35	6	2
1:B:704:LEU:HD12	1:C:714:PRO:HA	0.42	1.91	9	1
1:A:768:TYR:CZ	1:C:802:TYR:CD2	0.42	3.06	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:819:ALA:HB1	1:A:826:THR:CB	0.42	2.44	12	1
1:C:756:ILE:H	1:C:756:ILE:HD13	0.42	1.74	12	1
1:B:704:LEU:HD13	1:C:707:ARG:CB	0.42	2.44	13	1
1:C:675:ILE:HD11	1:C:678:TRP:CE3	0.42	2.49	15	1
1:A:746:ILE:O	1:A:749:VAL:HG23	0.42	2.13	14	2
1:C:670:TRP:N	1:C:670:TRP:CD1	0.42	2.87	3	1
1:B:791:GLU:HG2	1:C:753:LEU:HD13	0.42	1.92	5	1
1:C:770:ARG:O	1:C:774:LEU:N	0.42	2.52	12	1
1:B:771:LEU:HD21	1:B:772:ARG:HE	0.42	1.74	14	1
1:A:774:LEU:HD21	1:B:742:ARG:CZ	0.42	2.44	1	1
1:A:793:LEU:HD11	1:A:848:ARG:HB2	0.42	1.89	2	1
1:B:771:LEU:HD13	1:B:772:ARG:H	0.42	1.74	2	1
1:C:775:LEU:O	1:C:778:VAL:HG12	0.42	2.14	2	1
1:C:661:LEU:HD23	1:C:661:LEU:N	0.42	2.30	4	1
1:A:747:ARG:O	1:A:751:GLY:N	0.42	2.52	7	1
1:C:755:LEU:C	1:C:755:LEU:HD23	0.42	2.34	7	1
1:C:843:ILE:HD13	1:C:843:ILE:N	0.42	2.28	7	1
1:A:760:LEU:HD23	1:A:760:LEU:C	0.42	2.34	8	1
1:A:750:ASN:HB3	1:C:785:LEU:HD23	0.42	1.90	11	1
1:B:677:ASN:O	1:B:681:TYR:CZ	0.42	2.72	11	1
1:C:791:GLU:O	1:C:794:LYS:HD2	0.42	2.15	12	1
1:C:830:ILE:HG23	1:C:831:GLU:N	0.42	2.29	12	1
1:B:695:LEU:HD23	1:B:695:LEU:C	0.42	2.35	14	1
1:C:660:LEU:HD12	1:C:660:LEU:O	0.42	2.15	1	1
1:C:833:VAL:HG23	1:C:834:GLN:N	0.42	2.29	12	6
1:A:793:LEU:HD21	1:A:847:ILE:CG1	0.42	2.41	4	1
1:A:812:VAL:HG13	1:A:834:GLN:OE1	0.42	2.15	5	1
1:A:705:VAL:O	1:A:708:VAL:HG23	0.42	2.15	7	1
1:A:816:ASN:CB	1:A:830:ILE:HD11	0.42	2.44	7	1
1:A:675:ILE:HD12	1:A:679:LEU:HD21	0.42	1.90	9	1
1:C:855:LEU:HD12	1:C:855:LEU:C	0.42	2.35	9	1
1:C:753:LEU:O	1:C:756:ILE:HG22	0.42	2.15	14	1
1:C:771:LEU:C	1:C:771:LEU:HD12	0.42	2.34	14	1
1:C:688:ILE:HD12	1:C:688:ILE:N	0.42	2.29	1	1
1:A:803:TRP:CH2	1:B:768:TYR:CZ	0.42	3.06	3	1
1:B:830:ILE:HG23	1:B:831:GLU:N	0.42	2.29	10	4
1:A:757:TRP:CD1	1:A:757:TRP:C	0.42	2.92	4	1
1:C:771:LEU:C	1:C:771:LEU:HD22	0.42	2.35	4	1
1:C:820:ILE:HD13	1:C:820:ILE:N	0.42	2.30	6	1
1:A:751:GLY:HA2	1:B:715:LEU:HD11	0.42	1.90	9	1
1:C:748:LEU:HD13	1:C:748:LEU:C	0.42	2.35	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:688:ILE:HD12	1:A:688:ILE:H	0.42	1.74	2	1
1:B:799:LEU:HD23	1:B:800:LEU:H	0.42	1.72	2	1
1:C:840:ILE:HA	1:C:843:ILE:HD11	0.42	1.90	2	1
1:A:822:VAL:HG13	1:A:823:GLY:N	0.42	2.29	13	1
1:B:765:LEU:C	1:B:765:LEU:HD12	0.42	2.35	1	1
1:C:781:ILE:HG22	1:C:785:LEU:CD1	0.42	2.45	3	1
1:A:748:LEU:C	1:A:748:LEU:HD13	0.42	2.34	6	1
1:A:795:TYR:CE1	1:B:756:ILE:HD13	0.42	2.50	6	1
1:B:708:VAL:HG12	1:B:741:ASP:HB2	0.42	1.92	10	1
1:B:821:ALA:O	1:B:822:VAL:HG22	0.42	2.15	10	1
1:C:764:SER:HB3	1:C:771:LEU:HD12	0.42	1.91	13	1
1:A:760:LEU:HD22	1:A:763:LEU:HD21	0.42	1.90	14	1
1:A:771:LEU:H	1:A:771:LEU:HD22	0.42	1.75	14	1
1:C:832:VAL:HG23	1:C:833:VAL:N	0.42	2.30	14	2
1:A:785:LEU:C	1:A:785:LEU:HD12	0.42	2.35	4	1
1:B:749:VAL:HG23	1:B:750:ASN:N	0.42	2.30	6	1
1:C:708:VAL:HG12	1:C:741:ASP:HB2	0.42	1.91	9	1
1:A:704:LEU:HD12	1:B:710:GLN:OE1	0.42	2.15	10	1
1:B:795:TYR:O	1:B:799:LEU:CD2	0.42	2.68	10	1
1:B:775:LEU:HD13	1:B:775:LEU:C	0.42	2.35	11	1
1:A:747:ARG:HA	1:A:750:ASN:HD21	0.42	1.74	14	1
1:A:843:ILE:HD13	1:A:844:PRO:N	0.42	2.30	15	1
1:A:714:PRO:HB3	1:C:748:LEU:HD13	0.42	1.92	1	1
1:B:775:LEU:O	1:B:778:VAL:HG12	0.42	2.15	2	1
1:A:753:LEU:O	1:A:756:ILE:HG12	0.42	2.15	4	1
1:A:756:ILE:O	1:A:760:LEU:CD2	0.42	2.68	4	1
1:B:841:ARG:O	1:B:842:HIS:C	0.42	2.58	4	1
1:B:808:LYS:O	1:B:812:VAL:HG13	0.42	2.14	6	1
1:C:695:LEU:HD23	1:C:695:LEU:C	0.42	2.35	8	1
1:B:774:LEU:O	1:B:777:ILE:HG23	0.42	2.15	11	1
1:A:796:TRP:CD1	1:A:799:LEU:HD21	0.42	2.49	12	1
1:B:777:ILE:HD13	1:B:777:ILE:C	0.42	2.34	12	1
1:A:771:LEU:HD21	1:C:806:GLU:OE1	0.42	2.14	13	1
1:A:754:ALA:CB	1:B:715:LEU:HD22	0.42	2.45	14	1
1:B:778:VAL:HG23	1:C:746:ILE:HD11	0.42	1.92	2	1
1:A:753:LEU:HD13	1:C:791:GLU:HB3	0.42	1.91	8	1
1:C:760:LEU:C	1:C:760:LEU:HD23	0.42	2.35	8	1
1:B:748:LEU:HD23	1:C:714:PRO:HB3	0.42	1.91	10	1
1:A:753:LEU:HD12	1:A:754:ALA:N	0.42	2.30	12	1
1:A:829:VAL:O	1:A:833:VAL:HG23	0.41	2.15	2	1
1:A:785:LEU:HD21	1:B:746:ILE:CG2	0.41	2.45	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:806:GLU:HG3	1:B:771:LEU:HD21	0.41	1.91	5	1
1:C:715:LEU:HD23	1:C:715:LEU:O	0.41	2.14	5	1
1:C:822:VAL:HG23	1:C:823:GLY:N	0.41	2.30	8	1
1:B:672:TRP:CD1	1:B:672:TRP:N	0.41	2.88	12	2
1:A:748:LEU:HD23	1:A:748:LEU:C	0.41	2.35	11	1
1:A:760:LEU:C	1:A:760:LEU:HD22	0.41	2.35	12	1
1:A:791:GLU:HB2	1:B:753:LEU:HD22	0.41	1.92	12	1
1:A:746:ILE:HD12	1:A:746:ILE:N	0.41	2.29	3	2
1:B:820:ILE:HD12	1:B:820:ILE:N	0.41	2.30	7	2
1:C:750:ASN:ND2	1:C:750:ASN:H	0.41	2.13	3	1
1:C:822:VAL:HG13	1:C:822:VAL:O	0.41	2.15	4	1
1:A:795:TYR:O	1:B:756:ILE:HG21	0.41	2.15	5	2
1:A:764:SER:HB3	1:A:771:LEU:HD23	0.41	1.92	7	1
1:B:819:ALA:O	1:B:822:VAL:HG22	0.41	2.15	9	1
1:C:699:PHE:HA	1:C:702:LEU:HB3	0.41	1.92	9	2
1:B:748:LEU:C	1:B:748:LEU:HD23	0.41	2.35	14	1
1:A:812:VAL:HG23	1:A:813:SER:N	0.41	2.30	2	4
1:A:806:GLU:HG3	1:B:771:LEU:HD11	0.41	1.92	5	1
1:A:775:LEU:HD22	1:A:775:LEU:N	0.41	2.29	6	1
1:C:826:THR:O	1:C:830:ILE:HD13	0.41	2.15	6	1
1:A:710:GLN:HG2	1:A:715:LEU:HD22	0.41	1.90	9	1
1:A:696:ARG:HD2	1:C:697:ILE:HG22	0.41	1.91	10	1
1:B:675:ILE:HD12	1:B:675:ILE:C	0.41	2.34	12	1
1:C:702:LEU:HD22	1:C:702:LEU:C	0.41	2.36	12	1
1:C:774:LEU:HD13	1:C:774:LEU:C	0.41	2.35	12	1
1:A:814:LEU:O	1:A:814:LEU:HD13	0.41	2.15	15	1
1:C:710:GLN:OE1	1:C:715:LEU:HD22	0.41	2.16	1	1
1:B:796:TRP:HA	1:B:799:LEU:HD22	0.41	1.91	2	1
1:A:808:LYS:HE3	1:A:839:ALA:HB2	0.41	1.92	4	1
1:B:712:TYR:CG	1:B:713:SER:N	0.41	2.88	14	2
1:C:690:GLY:O	1:C:693:ILE:HG23	0.41	2.15	8	2
1:A:795:TYR:CD1	1:A:795:TYR:C	0.41	2.94	11	1
1:B:855:LEU:HD22	1:B:855:LEU:C	0.41	2.34	12	1
1:A:707:ARG:NH2	1:C:707:ARG:CZ	0.41	2.83	15	1
1:C:682:ILE:HD13	1:C:682:ILE:N	0.41	2.30	15	1
1:B:826:THR:O	1:B:829:VAL:HG12	0.41	2.15	4	1
1:A:708:VAL:HG21	1:B:714:PRO:HD2	0.41	1.93	5	1
1:B:686:ILE:HD12	1:B:686:ILE:N	0.41	2.30	6	1
1:C:745:SER:O	1:C:748:LEU:HD22	0.41	2.15	6	1
1:A:686:ILE:HG21	1:B:686:ILE:HD11	0.41	1.92	7	1
1:A:661:LEU:HD12	1:C:666:TRP:CG	0.41	2.50	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:820:ILE:N	1:C:820:ILE:HD12	0.41	2.30	11	1
1:A:704:LEU:HD21	1:B:707:ARG:HB2	0.41	1.92	6	1
1:A:714:PRO:O	1:C:704:LEU:HD21	0.41	2.16	3	1
1:A:771:LEU:HD12	1:A:771:LEU:C	0.41	2.36	3	1
1:A:795:TYR:CD2	1:B:753:LEU:O	0.41	2.74	3	1
1:A:803:TRP:CZ2	1:B:760:LEU:HD11	0.41	2.50	3	1
1:B:768:TYR:C	1:B:770:ARG:H	0.41	2.18	5	1
1:C:743:ASP:O	1:C:746:ILE:HG22	0.41	2.15	5	1
1:C:836:ALA:O	1:C:840:ILE:HD12	0.41	2.15	7	1
1:B:794:LYS:CD	1:B:795:TYR:N	0.41	2.84	8	1
1:A:661:LEU:HD12	1:C:666:TRP:CD2	0.41	2.51	11	1
1:C:854:ILE:HD13	1:C:854:ILE:O	0.41	2.16	12	1
1:A:663:LEU:HD23	1:B:660:LEU:O	0.41	2.16	14	1
1:C:699:PHE:O	1:C:702:LEU:HB3	0.41	2.16	1	2
1:A:707:ARG:HB2	1:C:704:LEU:HD21	0.41	1.93	2	1
1:A:756:ILE:O	1:A:760:LEU:CB	0.41	2.68	2	1
1:B:763:LEU:HD23	1:B:763:LEU:C	0.41	2.36	6	2
1:C:816:ASN:OD1	1:C:816:ASN:N	0.41	2.53	3	1
1:B:821:ALA:C	1:B:822:VAL:HG22	0.41	2.36	4	1
1:A:792:ALA:O	1:A:795:TYR:HD2	0.41	1.98	10	3
1:A:816:ASN:O	1:A:827:ASP:OD2	0.41	2.38	10	1
1:B:847:ILE:HD13	1:B:847:ILE:N	0.41	2.30	14	1
1:A:677:ASN:O	1:A:681:TYR:CZ	0.41	2.74	2	1
1:C:715:LEU:HD13	1:C:715:LEU:C	0.41	2.35	2	1
1:A:760:LEU:HD11	1:C:803:TRP:CH2	0.41	2.49	3	1
1:B:781:ILE:HD12	1:C:746:ILE:CB	0.41	2.45	3	1
1:B:814:LEU:HD13	1:B:814:LEU:C	0.41	2.36	4	1
1:B:847:ILE:HG23	1:B:848:ARG:N	0.41	2.31	9	2
1:C:678:TRP:CD1	1:C:678:TRP:C	0.41	2.94	4	1
1:A:742:ARG:NH2	1:C:774:LEU:HD21	0.41	2.31	5	1
1:B:667:ALA:HB2	1:C:660:LEU:HD22	0.41	1.91	5	1
1:A:747:ARG:O	1:A:747:ARG:CD	0.41	2.69	7	1
1:A:774:LEU:HD23	1:A:774:LEU:C	0.41	2.36	9	1
1:A:851:LEU:HD22	1:A:854:ILE:HD11	0.41	1.92	9	1
1:C:750:ASN:H	1:C:750:ASN:ND2	0.41	2.14	9	1
1:B:760:LEU:O	1:B:763:LEU:HD13	0.41	2.16	10	1
1:B:753:LEU:HD12	1:B:753:LEU:H	0.41	1.76	11	1
1:B:775:LEU:HD22	1:B:775:LEU:C	0.41	2.36	11	1
1:C:704:LEU:O	1:C:707:ARG:HB3	0.41	2.16	12	1
1:B:803:TRP:CE3	1:C:768:TYR:CE2	0.41	3.09	13	1
1:A:660:LEU:N	1:A:660:LEU:HD22	0.41	2.31	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:776:LEU:HD12	1:B:777:ILE:N	0.41	2.31	14	1
1:A:746:ILE:HG22	1:C:785:LEU:HD22	0.41	1.92	1	1
1:C:768:TYR:O	1:C:769:HIS:CB	0.41	2.69	2	1
1:A:753:LEU:HD22	1:C:791:GLU:HB2	0.41	1.92	3	1
1:A:675:ILE:HD13	1:A:675:ILE:C	0.41	2.36	5	2
1:C:774:LEU:O	1:C:777:ILE:HG22	0.41	2.15	6	1
1:A:806:GLU:OE2	1:B:771:LEU:HD21	0.41	2.16	11	1
1:B:845:ARG:O	1:B:846:ARG:C	0.41	2.59	11	1
1:A:815:LEU:O	1:A:819:ALA:HB2	0.41	2.16	14	1
1:A:779:THR:O	1:A:782:VAL:HG22	0.41	2.15	15	1
1:A:746:ILE:HG21	1:C:781:ILE:HG21	0.40	1.93	9	2
1:C:679:LEU:HD23	1:C:679:LEU:O	0.40	2.16	1	1
1:A:756:ILE:HD12	1:A:756:ILE:H	0.40	1.76	6	1
1:A:760:LEU:HD21	1:C:799:LEU:HD12	0.40	1.93	7	1
1:B:765:LEU:HD13	1:B:774:LEU:HD11	0.40	1.92	9	1
1:C:698:VAL:HG23	1:C:699:PHE:CD2	0.40	2.49	12	1
1:B:821:ALA:O	1:B:822:VAL:CB	0.40	2.70	13	1
1:A:814:LEU:O	1:A:818:THR:HG22	0.40	2.16	2	1
1:A:760:LEU:HG	1:C:799:LEU:HD12	0.40	1.92	3	1
1:B:781:ILE:CD1	1:C:746:ILE:HG21	0.40	2.45	3	1
1:A:660:LEU:HG	1:C:667:ALA:HB2	0.40	1.91	7	1
1:B:799:LEU:HD21	1:C:760:LEU:HD12	0.40	1.93	7	1
1:A:808:LYS:O	1:A:812:VAL:HG12	0.40	2.16	8	1
1:B:758:ASP:O	1:B:761:ARG:CZ	0.40	2.69	10	1
1:A:693:ILE:HD11	1:B:692:LEU:HD23	0.40	1.93	11	1
1:A:754:ALA:HB3	1:B:715:LEU:CD2	0.40	2.47	15	1
1:A:793:LEU:HD12	1:A:797:TRP:CE2	0.40	2.51	15	1
1:A:836:ALA:O	1:A:840:ILE:HG22	0.40	2.17	15	1
1:B:755:LEU:CA	1:C:715:LEU:HD11	0.40	2.46	1	1
1:C:760:LEU:HD13	1:C:761:ARG:N	0.40	2.31	1	1
1:C:812:VAL:HG12	1:C:816:ASN:ND2	0.40	2.30	1	1
1:A:750:ASN:ND2	1:A:750:ASN:N	0.40	2.69	5	1
1:B:683:ARG:NH1	1:C:679:LEU:HD11	0.40	2.31	5	1
1:C:782:VAL:HA	1:C:785:LEU:HD11	0.40	1.93	6	1
1:A:803:TRP:O	1:A:806:GLU:HG3	0.40	2.15	7	1
1:B:822:VAL:HG23	1:B:823:GLY:N	0.40	2.32	9	1
1:C:847:ILE:HG13	1:C:848:ARG:H	0.40	1.76	10	1
1:C:843:ILE:H	1:C:844:PRO:CD	0.40	2.29	11	1
1:B:816:ASN:ND2	1:B:820:ILE:HD11	0.40	2.31	15	1
1:B:830:ILE:HD12	1:B:830:ILE:C	0.40	2.37	1	1
1:C:706:ASN:O	1:C:710:GLN:N	0.40	2.54	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:808:LYS:NZ	1:B:834:GLN:O	0.40	2.54	11	1
1:B:842:HIS:HB3	1:B:843:ILE:HD13	0.40	1.93	12	1
1:A:763:LEU:O	1:A:774:LEU:CB	0.40	2.70	15	1
1:A:678:TRP:CD1	1:A:679:LEU:N	0.40	2.90	2	1
1:A:694:GLY:O	1:A:697:ILE:HG13	0.40	2.16	6	1
1:C:790:TRP:CH2	1:C:793:LEU:HD22	0.40	2.51	6	1
1:C:802:TYR:HB3	1:C:803:TRP:CZ3	0.40	2.52	6	1
1:C:682:ILE:HD13	1:C:683:ARG:N	0.40	2.31	8	1
1:B:795:TYR:O	1:B:799:LEU:HD23	0.40	2.16	10	1
1:C:746:ILE:O	1:C:749:VAL:HG23	0.40	2.16	10	1
1:C:663:LEU:HD22	1:C:664:ASP:N	0.40	2.30	12	1

## 6.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	171/197 (87%)	154±2 (90±1%)	10±2 (6±1%)	7±2 (4±1%)	5	32
1	B	171/197 (87%)	152±2 (89±1%)	10±2 (6±1%)	8±2 (5±1%)	4	26
1	C	171/197 (87%)	154±2 (90±1%)	10±2 (6±1%)	7±3 (4±2%)	5	31
All	All	7695/8865 (87%)	6905 (90%)	459 (6%)	331 (4%)	5	29

All 68 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	714	PRO	15
1	C	714	PRO	15
1	B	714	PRO	14
1	C	712	TYR	11
1	A	741	ASP	9
1	B	673	PHE	9
1	C	673	PHE	9
1	B	765	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	C	767	SER	8
1	C	843	ILE	8
1	B	846	ARG	8
1	A	825	GLY	7
1	C	661	LEU	7
1	B	824	GLU	7
1	B	842	HIS	7
1	B	844	PRO	7
1	C	769	HIS	7
1	A	673	PHE	6
1	A	768	TYR	6
1	C	765	LEU	6
1	C	822	VAL	6
1	A	661	LEU	6
1	B	712	TYR	6
1	B	661	LEU	5
1	C	766	PHE	5
1	A	822	VAL	5
1	B	674	ASP	5
1	B	766	PHE	5
1	B	825	GLY	5
1	A	712	TYR	5
1	A	769	HIS	5
1	A	846	ARG	5
1	B	767	SER	5
1	B	822	VAL	5
1	A	765	LEU	4
1	B	663	LEU	4
1	B	769	HIS	4
1	C	674	ASP	4
1	C	821	ALA	4
1	A	821	ALA	4
1	B	662	GLU	4
1	B	768	TYR	4
1	B	821	ALA	4
1	A	662	GLU	4
1	C	824	GLU	4
1	A	824	GLU	4
1	A	674	ASP	3
1	A	843	ILE	3
1	A	767	SER	2
1	B	845	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	B	843	ILE	2
1	C	846	ARG	2
1	A	766	PHE	2
1	B	823	GLY	2
1	A	844	PRO	2
1	A	845	ARG	2
1	C	823	GLY	2
1	C	768	TYR	2
1	B	741	ASP	1
1	C	662	GLU	1
1	B	715	LEU	1
1	B	711	GLY	1
1	A	823	GLY	1
1	C	844	PRO	1
1	A	715	LEU	1
1	C	825	GLY	1
1	C	663	LEU	1
1	C	715	LEU	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	155/173 (90%)	116±6 (75±4%)	39±6 (25±4%)	2	25
1	B	155/173 (90%)	117±6 (76±4%)	38±6 (24±4%)	2	26
1	C	155/173 (90%)	115±5 (74±3%)	40±5 (26±3%)	2	23
All	All	6975/7785 (90%)	5231 (75%)	1744 (25%)	2	25

All 409 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	803	TRP	15
1	B	803	TRP	15
1	C	771	LEU	15
1	C	794	LYS	15
1	C	803	TRP	15

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Mol	Chain	Res	Type	Models (Total)
1	B	794	LYS	14
1	A	744	ARG	13
1	A	771	LEU	13
1	B	771	LEU	13
1	A	678	TRP	12
1	A	763	LEU	12
1	A	794	LYS	12
1	B	744	ARG	12
1	C	761	ARG	12
1	C	795	TYR	12
1	A	715	LEU	11
1	A	795	TYR	11
1	B	834	GLN	11
1	C	678	TRP	11
1	A	693	ILE	11
1	A	780	ARG	11
1	B	678	TRP	11
1	C	799	LEU	11
1	A	753	LEU	10
1	A	770	ARG	10
1	B	763	LEU	10
1	B	772	ARG	10
1	C	693	ILE	10
1	C	744	ARG	10
1	C	757	TRP	10
1	C	774	LEU	10
1	C	775	LEU	10
1	A	830	ILE	10
1	B	675	ILE	10
1	C	696	ARG	10
1	C	715	LEU	10
1	A	679	LEU	10
1	A	772	ARG	9
1	A	838	ARG	9
1	B	702	LEU	9
1	B	715	LEU	9
1	B	774	LEU	9
1	B	795	TYR	9
1	B	802	TYR	9
1	C	680	TRP	9
1	B	799	LEU	9
1	A	697	ILE	8

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Mol	Chain	Res	Type	Models (Total)
1	A	712	TYR	8
1	C	675	ILE	8
1	C	707	ARG	8
1	C	758	ASP	8
1	C	780	ARG	8
1	C	838	ARG	8
1	C	847	ILE	8
1	A	692	LEU	8
1	B	693	ILE	8
1	C	663	LEU	8
1	C	764	SER	8
1	C	772	ARG	8
1	A	747	ARG	8
1	A	663	LEU	7
1	A	674	ASP	7
1	A	675	ILE	7
1	A	806	GLU	7
1	A	814	LEU	7
1	A	834	GLN	7
1	A	847	ILE	7
1	B	707	ARG	7
1	C	756	ILE	7
1	C	856	LEU	7
1	A	758	ASP	7
1	A	760	LEU	7
1	A	790	TRP	7
1	B	765	LEU	7
1	B	770	ARG	7
1	C	673	PHE	7
1	C	713	SER	7
1	C	748	LEU	7
1	A	765	LEU	7
1	B	805	GLN	7
1	B	847	ILE	7
1	A	662	GLU	6
1	A	757	TRP	6
1	B	674	ASP	6
1	B	708	VAL	6
1	B	760	LEU	6
1	B	767	SER	6
1	B	785	LEU	6
1	B	800	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	C	660	LEU	6
1	C	770	ARG	6
1	C	830	ILE	6
1	C	855	LEU	6
1	A	704	LEU	6
1	B	698	VAL	6
1	B	756	ILE	6
1	B	758	ASP	6
1	C	765	LEU	6
1	A	742	ARG	6
1	B	685	PHE	6
1	C	750	ASN	6
1	B	742	ARG	6
1	A	761	ARG	6
1	A	797	TRP	6
1	B	780	ARG	6
1	C	702	LEU	6
1	B	753	LEU	6
1	A	684	ILE	5
1	A	696	ARG	5
1	A	755	LEU	5
1	A	766	PHE	5
1	A	788	ARG	5
1	B	696	ARG	5
1	B	713	SER	5
1	B	775	LEU	5
1	B	781	ILE	5
1	B	830	ILE	5
1	B	846	ARG	5
1	C	682	ILE	5
1	C	697	ILE	5
1	C	706	ASN	5
1	C	760	LEU	5
1	C	802	TYR	5
1	C	841	ARG	5
1	C	846	ARG	5
1	C	848	ARG	5
1	A	660	LEU	5
1	A	785	LEU	5
1	A	799	LEU	5
1	A	856	LEU	5
1	B	679	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	B	757	TRP	5
1	B	801	GLN	5
1	B	855	LEU	5
1	B	856	LEU	5
1	C	763	LEU	5
1	C	779	THR	5
1	A	739	GLU	5
1	A	828	ARG	5
1	B	755	LEU	5
1	B	773	ASP	5
1	A	793	LEU	5
1	B	837	SER	5
1	C	791	GLU	5
1	B	745	SER	5
1	B	750	ASN	5
1	C	753	LEU	5
1	C	787	ARG	5
1	B	672	TRP	5
1	C	747	ARG	5
1	A	710	GLN	4
1	A	741	ASP	4
1	A	805	GLN	4
1	B	743	ASP	4
1	B	791	GLU	4
1	B	824	GLU	4
1	B	845	ARG	4
1	B	852	GLU	4
1	C	661	LEU	4
1	C	679	LEU	4
1	C	686	ILE	4
1	C	692	LEU	4
1	C	740	ARG	4
1	C	766	PHE	4
1	C	784	LEU	4
1	C	793	LEU	4
1	C	805	GLN	4
1	C	824	GLU	4
1	A	764	SER	4
1	A	774	LEU	4
1	A	776	LEU	4
1	A	854	ILE	4
1	B	673	PHE	4

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Mol	Chain	Res	Type	Models (Total)
1	B	692	LEU	4
1	B	739	GLU	4
1	B	814	LEU	4
1	C	676	THR	4
1	C	704	LEU	4
1	A	673	PHE	4
1	A	852	GLU	4
1	B	853	ARG	4
1	C	800	LEU	4
1	C	845	ARG	4
1	A	703	SER	4
1	A	746	ILE	4
1	B	746	ILE	4
1	C	716	SER	4
1	C	785	LEU	4
1	C	834	GLN	4
1	A	707	ARG	4
1	A	750	ASN	4
1	B	766	PHE	4
1	B	816	ASN	4
1	C	849	GLN	4
1	A	845	ARG	4
1	B	790	TRP	4
1	B	806	GLU	4
1	C	710	GLN	4
1	A	669	LEU	3
1	A	808	LYS	3
1	A	841	ARG	3
1	B	704	LEU	3
1	B	793	LEU	3
1	B	809	ASN	3
1	C	662	GLU	3
1	C	746	ILE	3
1	C	768	TYR	3
1	C	782	VAL	3
1	C	801	GLN	3
1	C	852	GLU	3
1	A	713	SER	3
1	A	752	SER	3
1	A	775	LEU	3
1	B	677	ASN	3
1	B	686	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	B	706	ASN	3
1	B	778	VAL	3
1	C	683	ARG	3
1	A	827	ASP	3
1	B	697	ILE	3
1	B	807	LEU	3
1	B	827	ASP	3
1	C	767	SER	3
1	C	816	ASN	3
1	C	826	THR	3
1	A	702	LEU	3
1	A	851	LEU	3
1	B	682	ILE	3
1	B	748	LEU	3
1	B	788	ARG	3
1	B	826	THR	3
1	C	709	ARG	3
1	C	806	GLU	3
1	A	665	LYS	3
1	A	791	GLU	3
1	A	800	LEU	3
1	A	843	ILE	3
1	B	661	LEU	3
1	B	662	GLU	3
1	B	663	LEU	3
1	B	740	ARG	3
1	B	761	ARG	3
1	B	764	SER	3
1	B	787	ARG	3
1	B	848	ARG	3
1	C	671	ASN	3
1	C	703	SER	3
1	C	762	SER	3
1	C	809	ASN	3
1	A	787	ARG	3
1	A	846	ARG	3
1	C	714	PRO	3
1	C	752	SER	3
1	C	843	ILE	3
1	A	807	LEU	3
1	A	815	LEU	3
1	B	660	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	C	743	ASP	3
1	C	790	TRP	3
1	A	769	HIS	3
1	A	677	ASN	3
1	B	777	ILE	3
1	A	767	SER	2
1	A	773	ASP	2
1	A	802	TYR	2
1	A	824	GLU	2
1	A	840	ILE	2
1	B	812	VAL	2
1	C	674	ASP	2
1	C	712	TYR	2
1	C	853	ARG	2
1	A	701	VAL	2
1	A	748	LEU	2
1	A	782	VAL	2
1	A	822	VAL	2
1	B	712	TYR	2
1	B	769	HIS	2
1	B	840	ILE	2
1	C	742	ARG	2
1	C	755	LEU	2
1	C	773	ASP	2
1	C	827	ASP	2
1	A	685	PHE	2
1	A	848	ARG	2
1	A	849	GLN	2
1	B	776	LEU	2
1	C	759	ASP	2
1	C	776	LEU	2
1	C	820	ILE	2
1	C	840	ILE	2
1	A	683	ARG	2
1	A	691	SER	2
1	A	743	ASP	2
1	B	701	VAL	2
1	B	808	LYS	2
1	B	838	ARG	2
1	C	769	HIS	2
1	C	851	LEU	2
1	A	768	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	B	669	LEU	2
1	B	762	SER	2
1	B	798	ASN	2
1	C	808	LYS	2
1	C	813	SER	2
1	A	664	ASP	2
1	A	676	THR	2
1	A	709	ARG	2
1	B	683	ARG	2
1	B	747	ARG	2
1	B	797	TRP	2
1	B	854	ILE	2
1	A	716	SER	2
1	A	777	ILE	2
1	B	699	PHE	2
1	C	691	SER	2
1	C	854	ILE	2
1	A	689	VAL	2
1	A	779	THR	2
1	A	801	GLN	2
1	B	842	HIS	2
1	C	664	ASP	2
1	C	739	GLU	2
1	B	710	GLN	2
1	B	783	GLU	2
1	B	784	LEU	2
1	C	781	ILE	2
1	A	809	ASN	2
1	B	815	LEU	2
1	B	828	ARG	2
1	C	705	VAL	2
1	A	855	LEU	2
1	B	843	ILE	2
1	A	671	ASN	2
1	A	708	VAL	2
1	C	807	LEU	2
1	B	841	ARG	2
1	A	820	ILE	1
1	B	671	ASN	1
1	C	684	ILE	1
1	A	810	SER	1
1	A	816	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	B	670	TRP	1
1	B	810	SER	1
1	C	669	LEU	1
1	C	822	VAL	1
1	A	714	PRO	1
1	A	781	ILE	1
1	C	670	TRP	1
1	C	677	ASN	1
1	C	699	PHE	1
1	C	708	VAL	1
1	C	783	GLU	1
1	B	714	PRO	1
1	B	752	SER	1
1	B	822	VAL	1
1	C	665	LYS	1
1	C	741	ASP	1
1	A	670	TRP	1
1	A	740	ARG	1
1	B	695	LEU	1
1	C	745	SER	1
1	C	804	SER	1
1	A	672	TRP	1
1	A	831	GLU	1
1	C	668	SER	1
1	C	831	GLU	1
1	A	661	LEU	1
1	B	691	SER	1
1	C	701	VAL	1
1	A	682	ILE	1
1	A	804	SER	1
1	B	782	VAL	1
1	C	815	LEU	1
1	B	716	SER	1
1	B	749	VAL	1
1	B	818	THR	1
1	B	851	LEU	1
1	C	695	LEU	1
1	C	778	VAL	1
1	C	788	ARG	1
1	C	797	TRP	1
1	C	810	SER	1
1	A	680	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	698	VAL	1
1	A	699	PHE	1
1	A	783	GLU	1
1	B	668	SER	1
1	B	688	ILE	1
1	C	672	TRP	1
1	C	698	VAL	1
1	A	686	ILE	1
1	B	680	TRP	1
1	C	818	THR	1
1	A	668	SER	1
1	A	706	ASN	1
1	B	676	THR	1
1	B	684	ILE	1
1	B	813	SER	1
1	C	842	HIS	1
1	A	842	HIS	1
1	A	853	ARG	1
1	B	831	GLU	1
1	A	688	ILE	1
1	A	756	ILE	1
1	A	762	SER	1
1	A	826	THR	1
1	A	837	SER	1
1	B	664	ASP	1
1	B	804	SER	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 9% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *HIV1\_gp41\_MPER-TMD-CT\_chemical\_shifts.tab*

#### 7.1.1 Bookkeeping

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

Total number of shifts	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	171	$-0.04 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	158	$-0.28 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	164	$0.90 \pm 0.26$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 9%, i.e. 622 atoms were assigned a chemical shift out of a possible 7095. 0 out of 132 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	622/2613 (24%)	156/1044 (15%)	310/1050 (30%)	156/519 (30%)
Sidechain	0/3846 (0%)	0/2235 (0%)	0/1377 (0%)	0/234 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/636 (0%)	0/324 (0%)	0/270 (0%)	0/42 (0%)
Overall	622/7095 (9%)	156/3603 (4%)	310/2697 (11%)	156/795 (20%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 622 atoms were assigned a chemical shift out of a possible 7095. 0 out of 132 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	622/2613 (24%)	156/1044 (15%)	310/1050 (30%)	156/519 (30%)
Sidechain	0/3846 (0%)	0/2235 (0%)	0/1377 (0%)	0/234 (0%)
Aromatic	0/636 (0%)	0/324 (0%)	0/270 (0%)	0/42 (0%)
Overall	622/7095 (9%)	156/3603 (4%)	310/2697 (11%)	156/795 (20%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

