



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 22, 2021 – 08:08 AM EDT

PDB ID : 7LOH  
Title : Structure of the HIV-1 gp41 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

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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

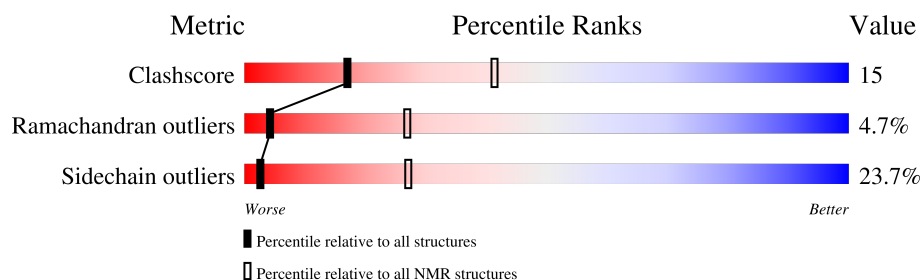
# 1 Overall quality at a glance

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	180	
1	B	180	
1	C	180	

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 5 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:692-A:716, A:739-A:856, B:689-B:716, B:739-B:856, C:690-C:716, C:739-C:856 (434)	0.82	5

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8049 atoms, of which 4131 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					Trace
1	A	158	Total	C	H	N	O	0
			2683	844	1377	245	217	
1	B	158	Total	C	H	N	O	0
			2683	844	1377	245	217	
1	C	158	Total	C	H	N	O	0
			2683	844	1377	245	217	

There are 24 discrepancies between the modelled and reference sequences:

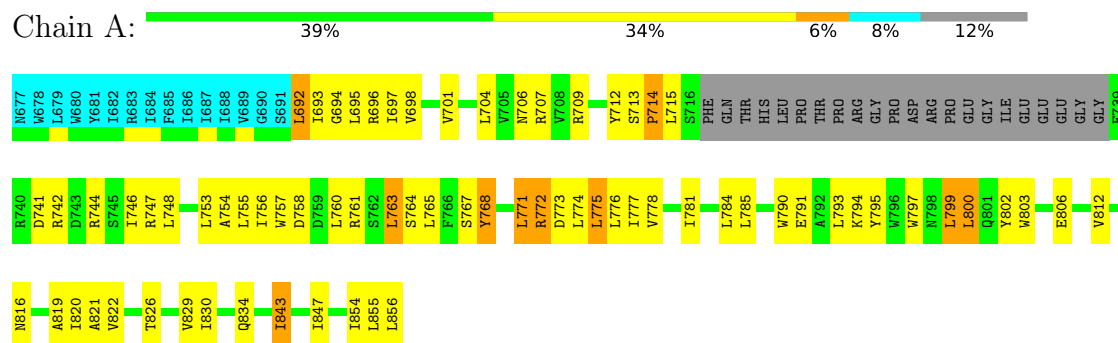
Chain	Residue	Modelled	Actual	Comment	Reference
A	683	ARG	LYS	conflict	UNP A0A386YSI0
A	687	ILE	MET	conflict	UNP A0A386YSI0
A	691	SER	GLY	conflict	UNP A0A386YSI0
A	693	ILE	VAL	conflict	UNP A0A386YSI0
A	704	LEU	ILE	conflict	UNP A0A386YSI0
A	764	SER	CYS	engineered mutation	UNP A0A386YSI0
A	823	GLY	ALA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

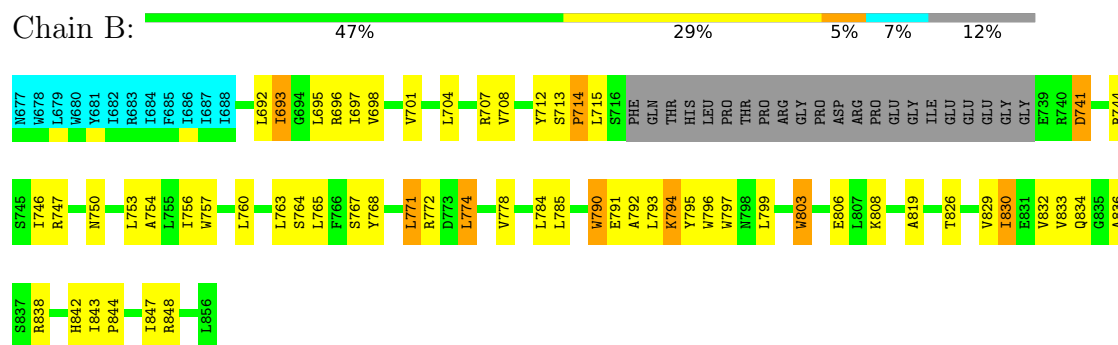
### 4.1 Average score per residue in the NMR ensemble

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.

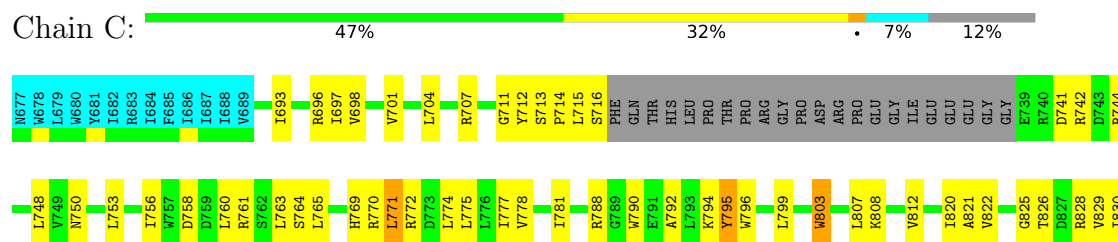
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41



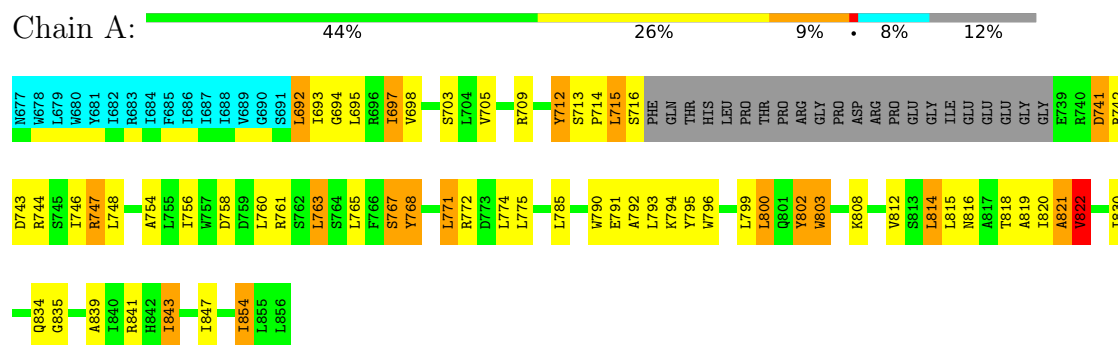


## 4.2 Scores per residue for each member of the ensemble

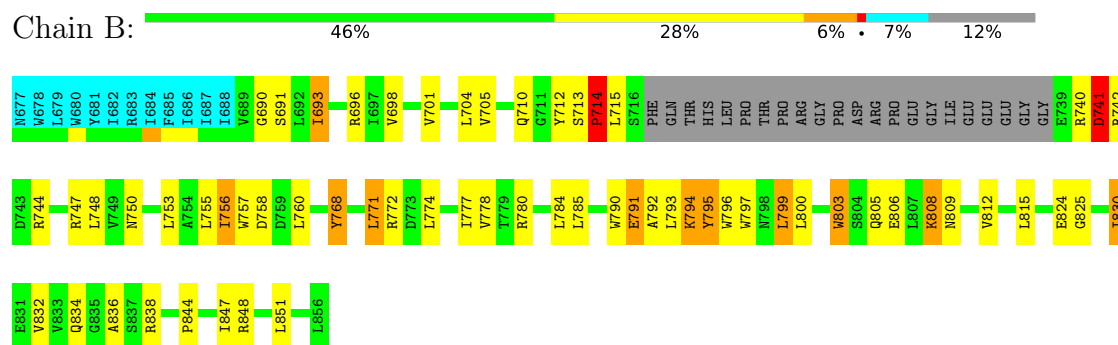
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

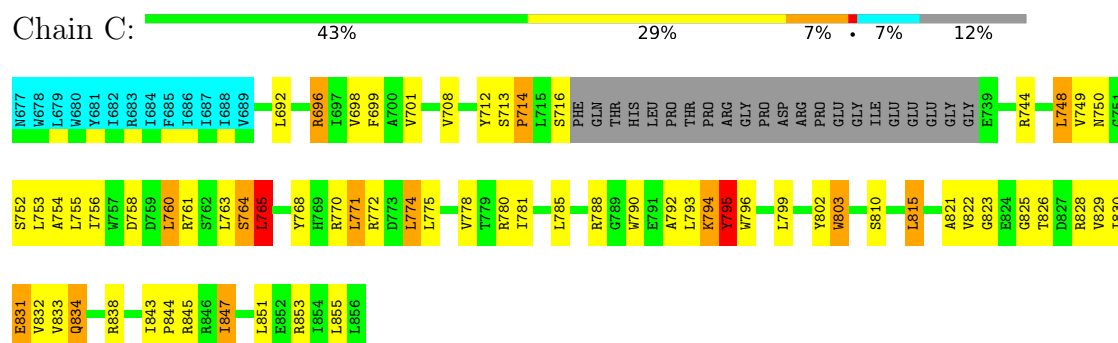
- Molecule 1: Transmembrane protein gp41



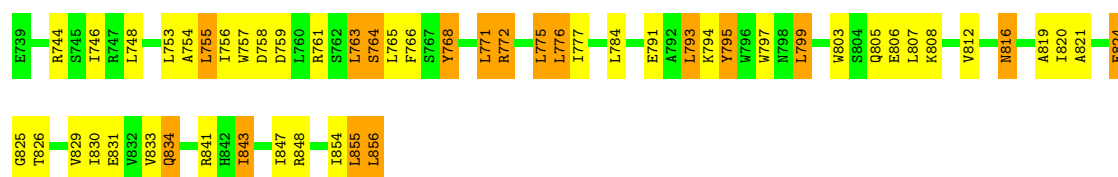
- Molecule 1: Transmembrane protein gp41



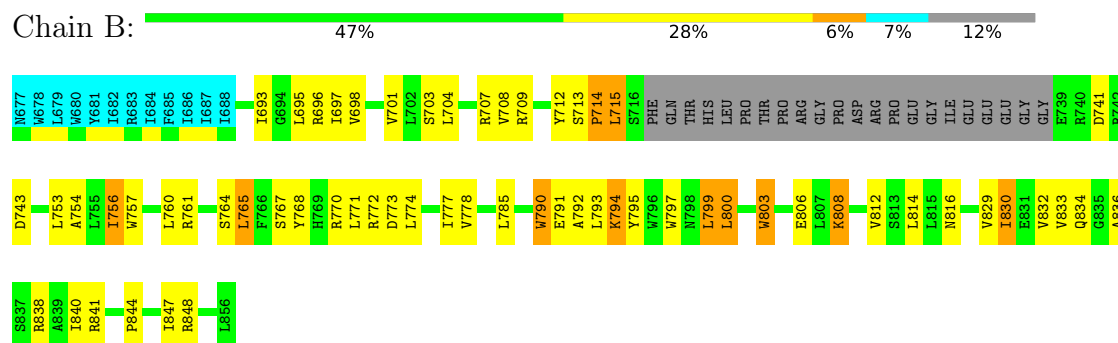
- Molecule 1: Transmembrane protein gp41



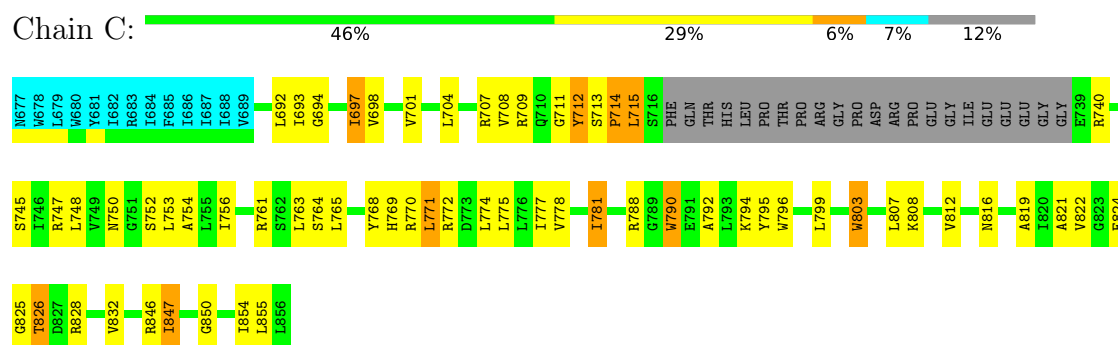




• Molecule 1: Transmembrane protein gp41

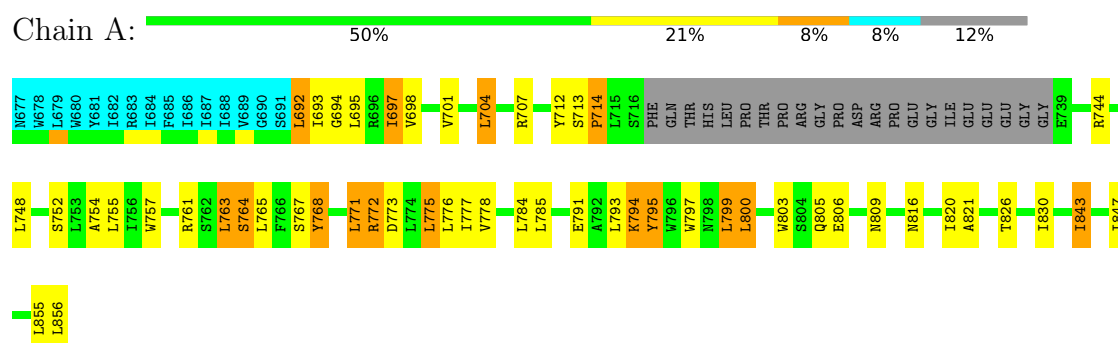


• Molecule 1: Transmembrane protein gp41



#### 4.2.4 Score per residue for model 4

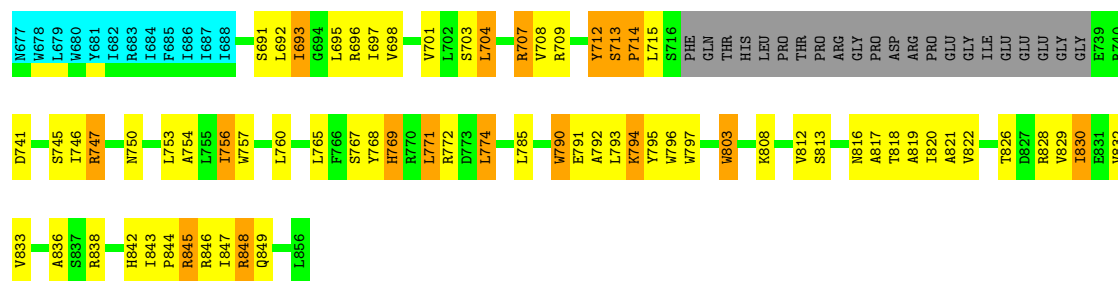
• Molecule 1: Transmembrane protein gp41



• Molecule 1: Transmembrane protein gp41

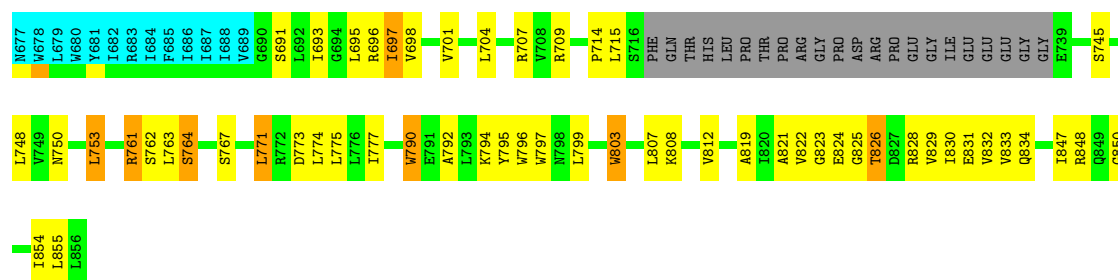






- Molecule 1: Transmembrane protein gp41

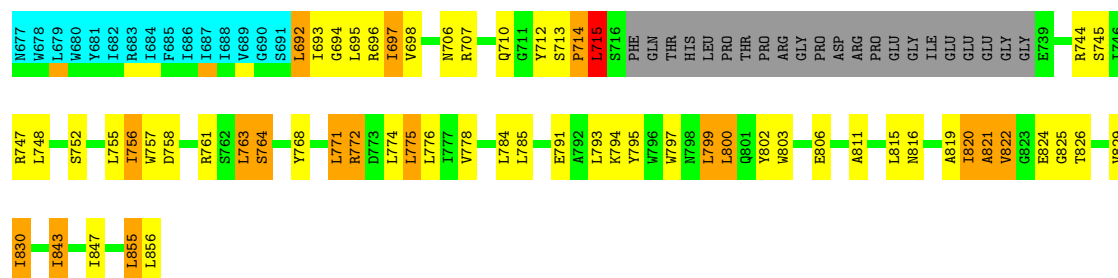
Chain C: 49% 27% 7% 12%



#### 4.2.5 Score per residue for model 5 (medoid)

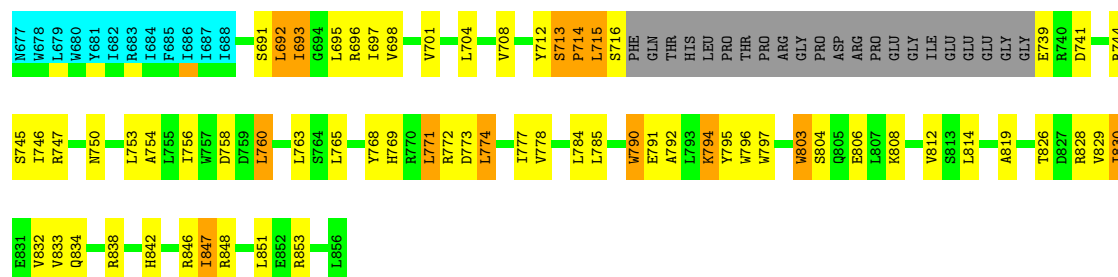
- Molecule 1: Transmembrane protein gp41

Chain A: 46% 24% 9% 8% 12%

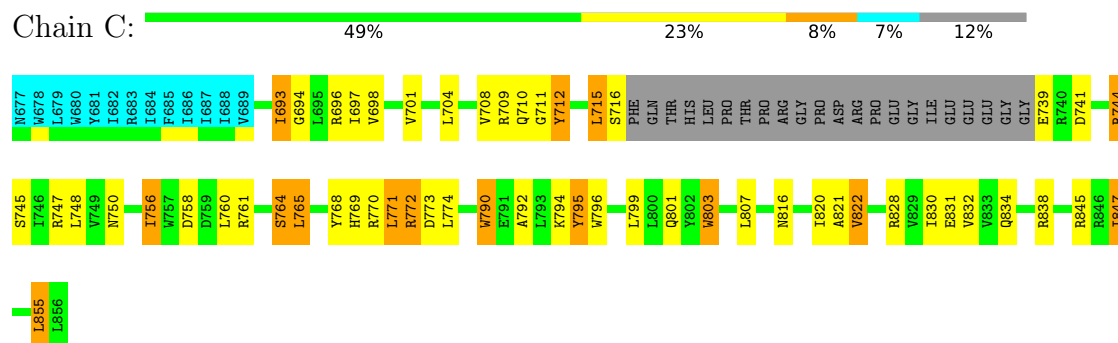


- Molecule 1: Transmembrane protein gp41

Chain B: 44% 30% 7% 7% 12%

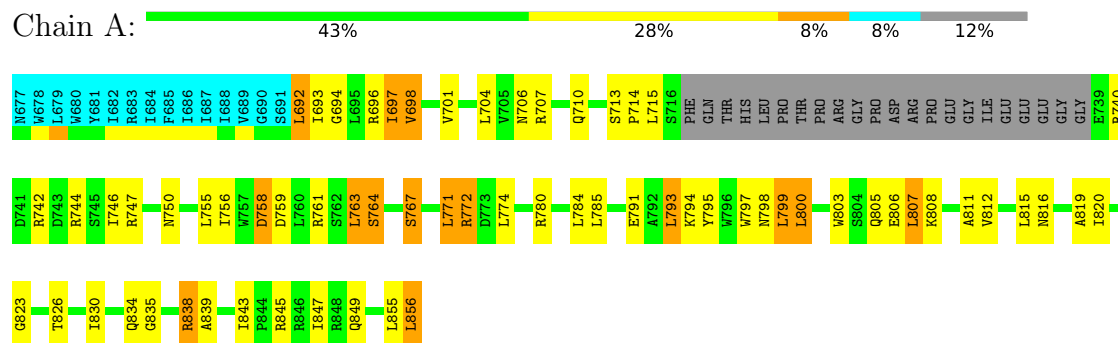


- Molecule 1: Transmembrane protein gp41

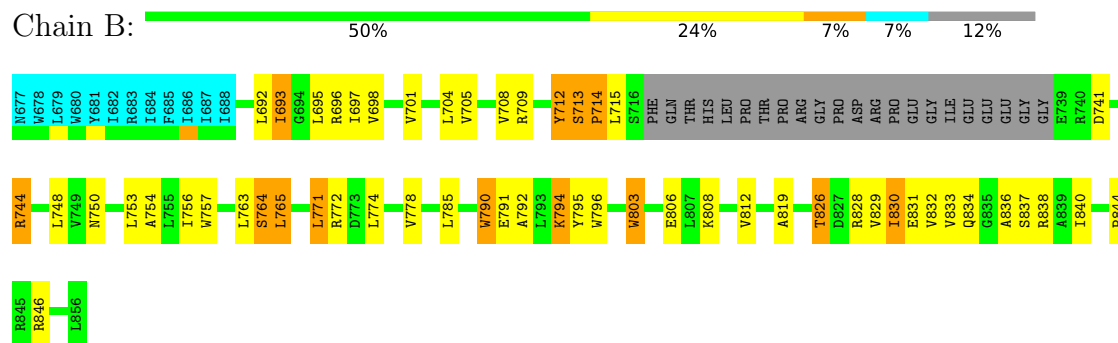


#### 4.2.6 Score per residue for model 6

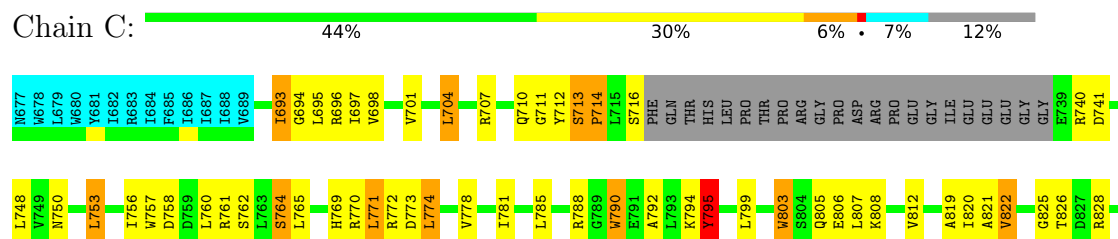
- Molecule 1: Transmembrane protein gp41

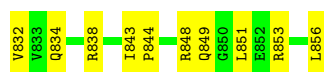


- Molecule 1: Transmembrane protein gp41



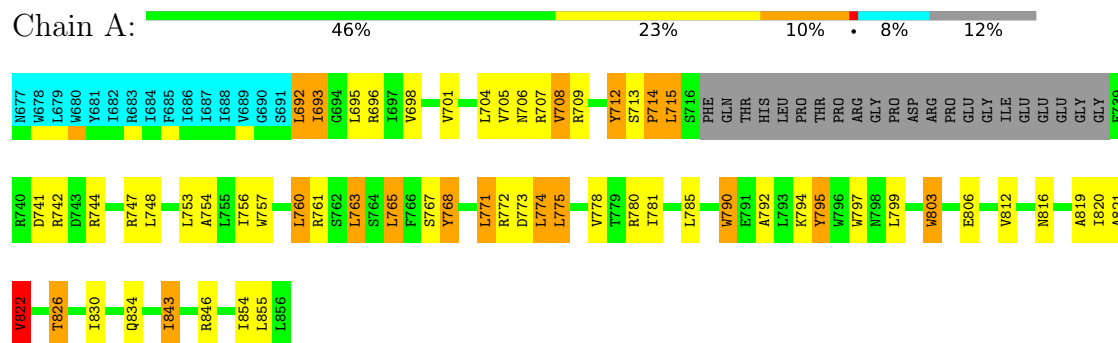
- Molecule 1: Transmembrane protein gp41



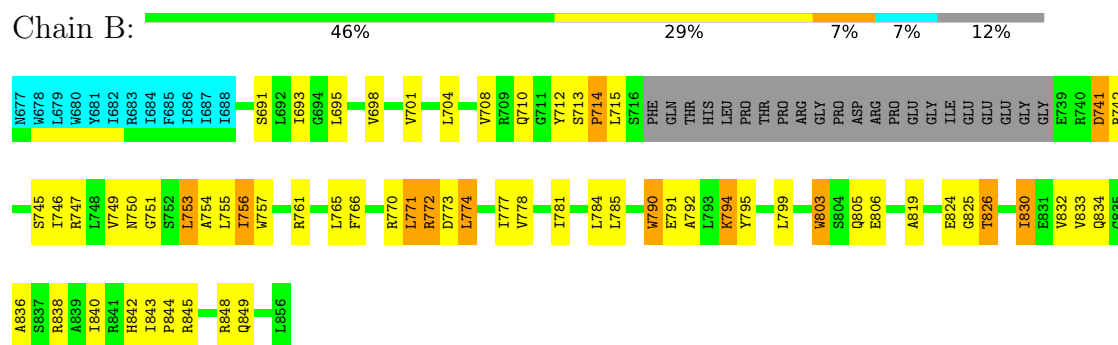


#### 4.2.7 Score per residue for model 7

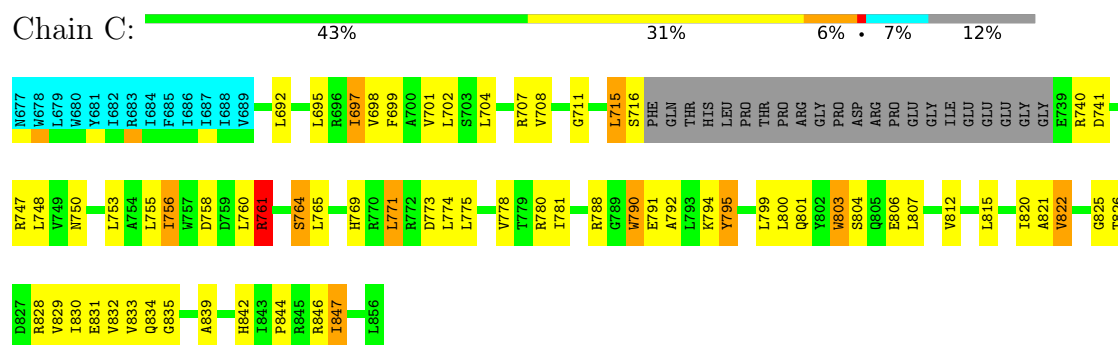
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

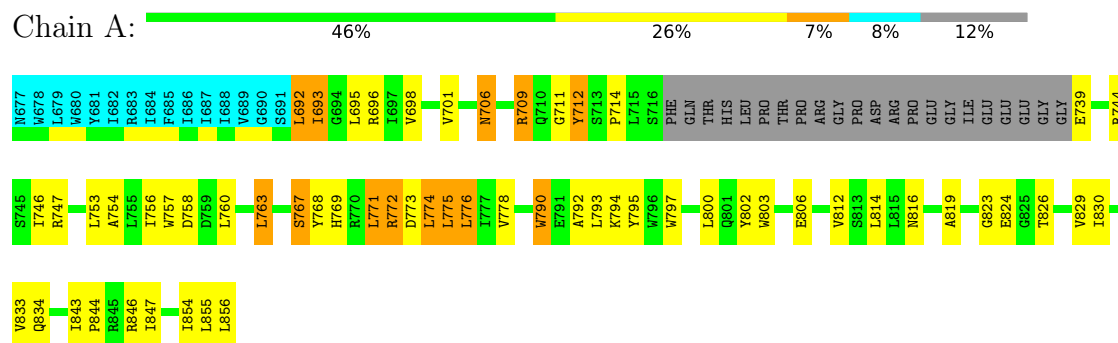


- Molecule 1: Transmembrane protein gp41

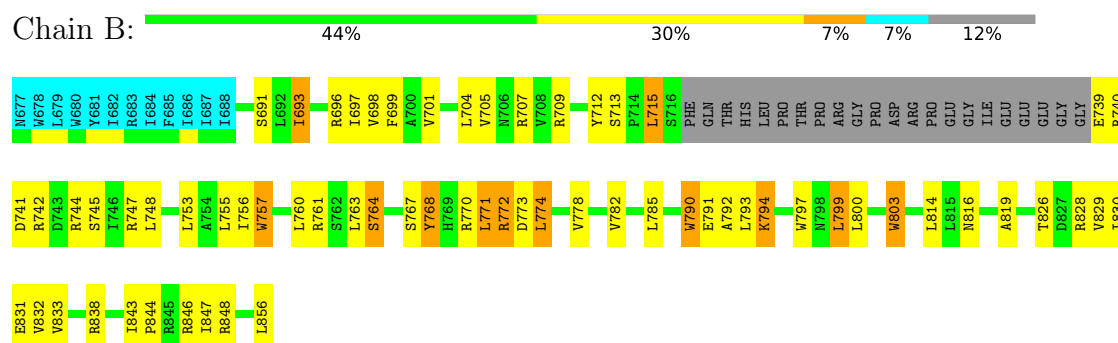


#### 4.2.8 Score per residue for model 8

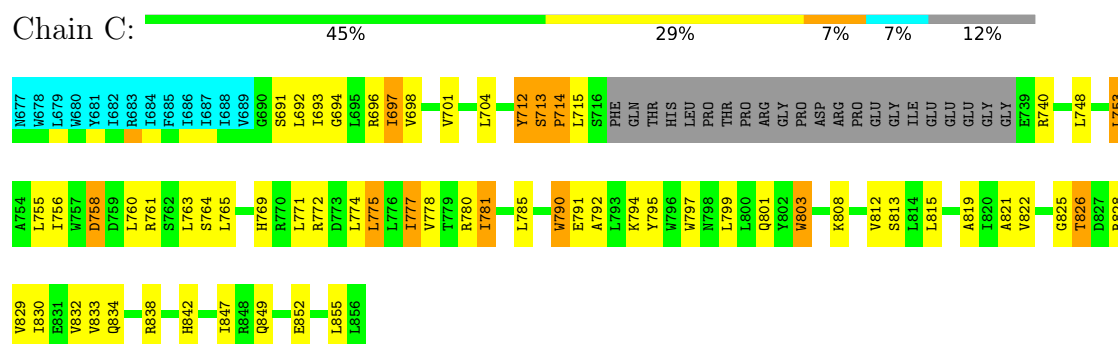
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

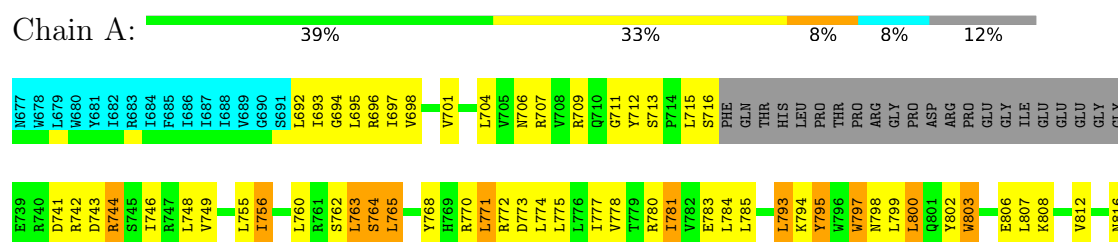


- Molecule 1: Transmembrane protein gp41



#### 4.2.9 Score per residue for model 9

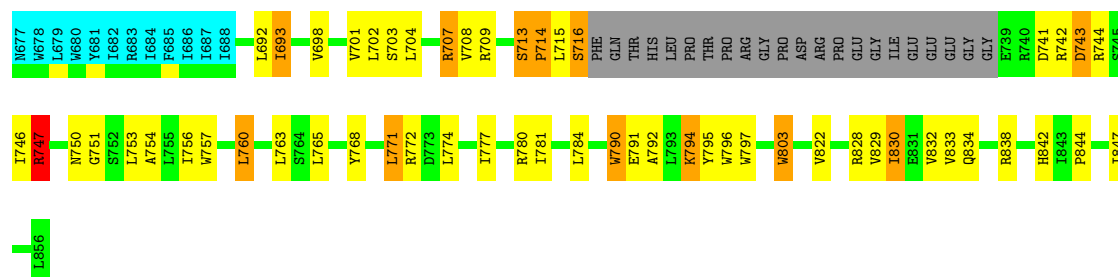
- Molecule 1: Transmembrane protein gp41





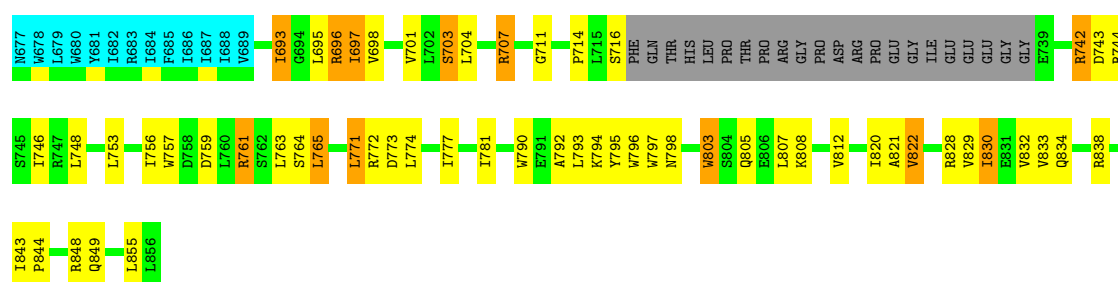
• Molecule 1: Transmembrane protein gp41

Chain B: 50% 24% 7% 7% 12%



• Molecule 1: Transmembrane protein gp41

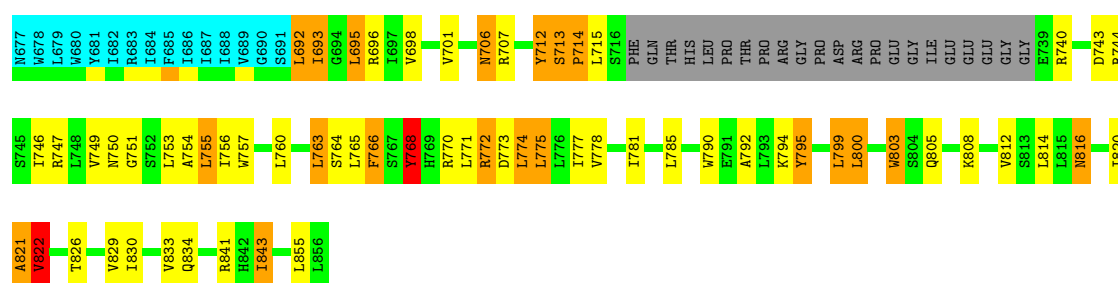
Chain C: 48% 26% 7% 7% 12%



#### 4.2.10 Score per residue for model 10

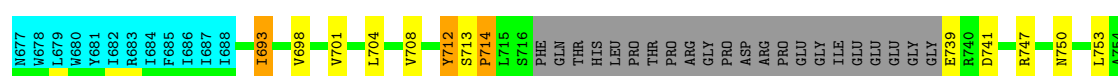
• Molecule 1: Transmembrane protein gp41

Chain A: 44% 23% 11% 8% 12%



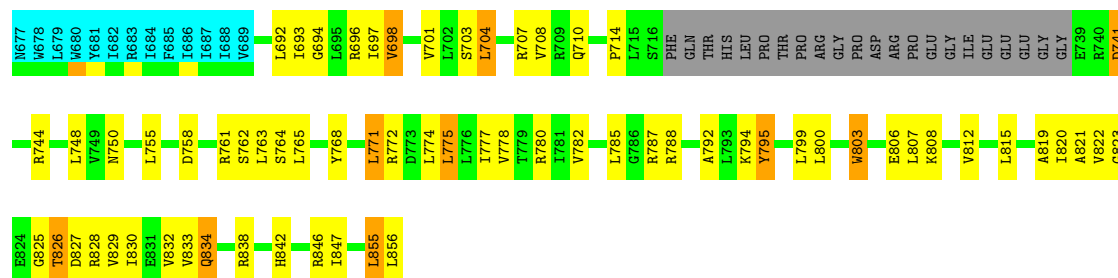
• Molecule 1: Transmembrane protein gp41

Chain B: 47% 27% 7% 7% 12%



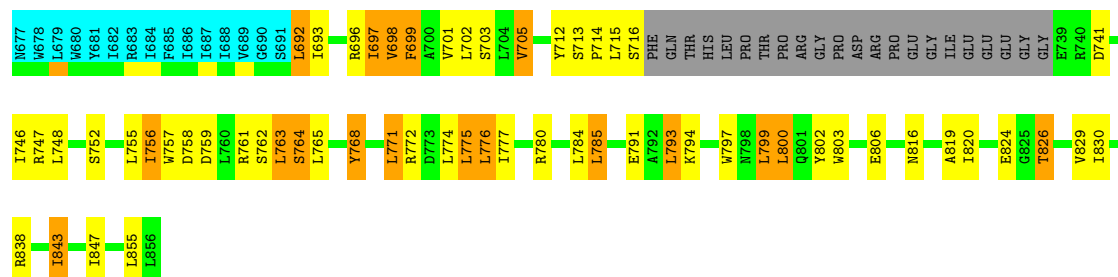


- Molecule 1: Transmembrane protein gp41

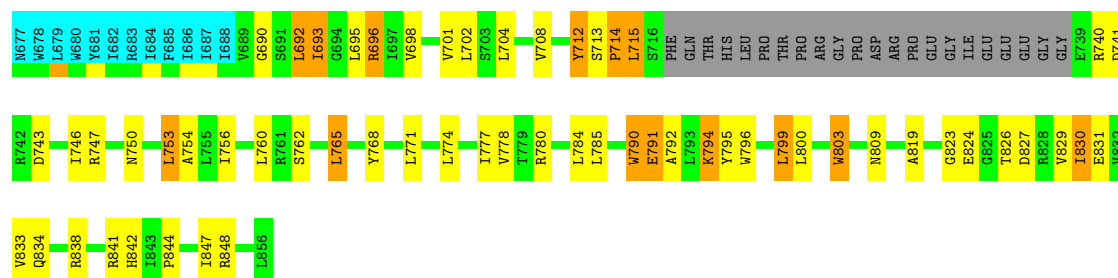


#### 4.2.11 Score per residue for model 11

- Molecule 1: Transmembrane protein gp41

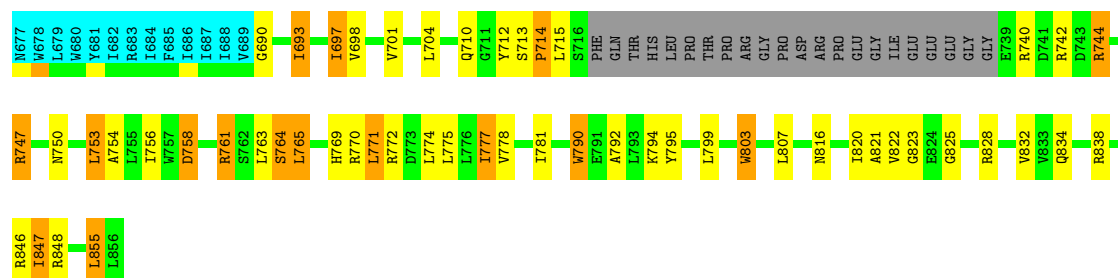


- Molecule 1: Transmembrane protein gp41



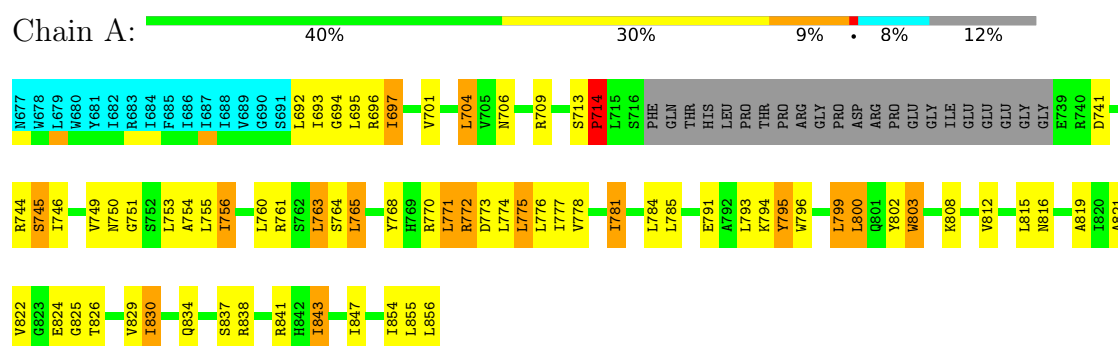
- Molecule 1: Transmembrane protein gp41



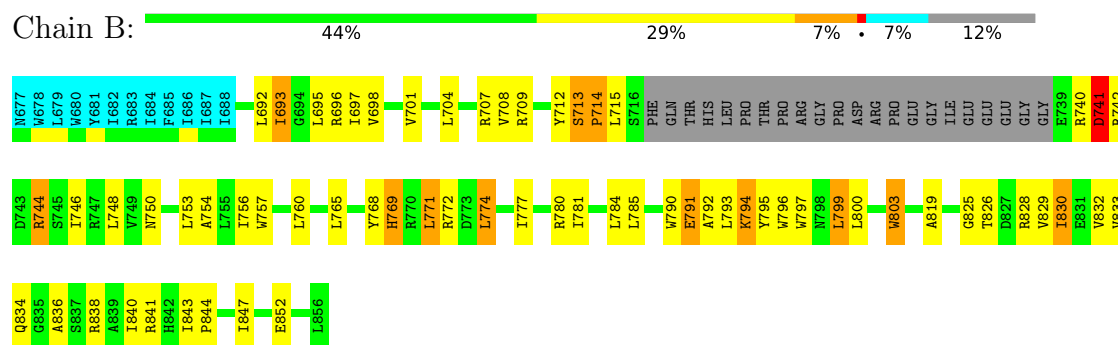


#### 4.2.12 Score per residue for model 12

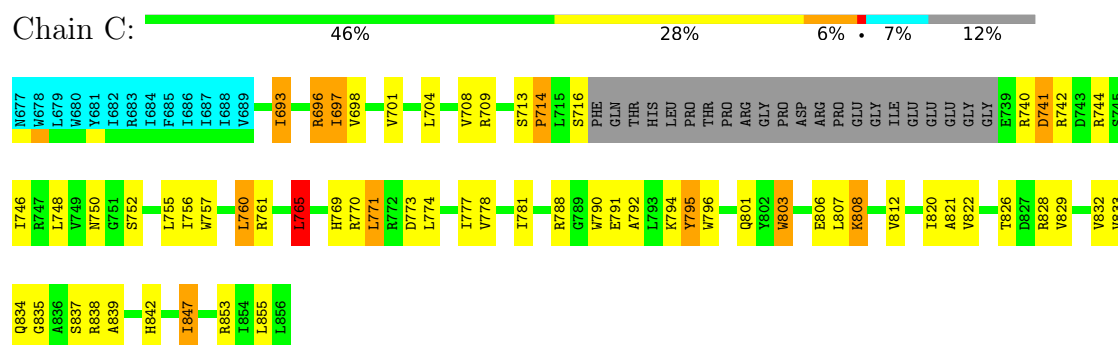
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

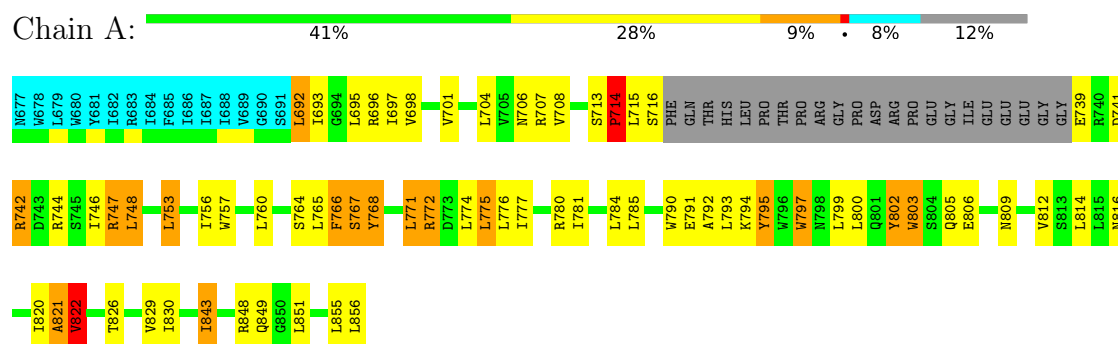


- Molecule 1: Transmembrane protein gp41

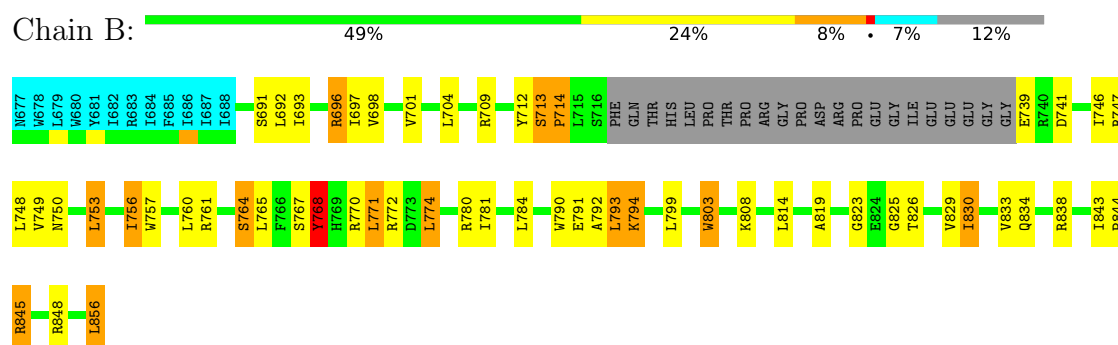


#### 4.2.13 Score per residue for model 13

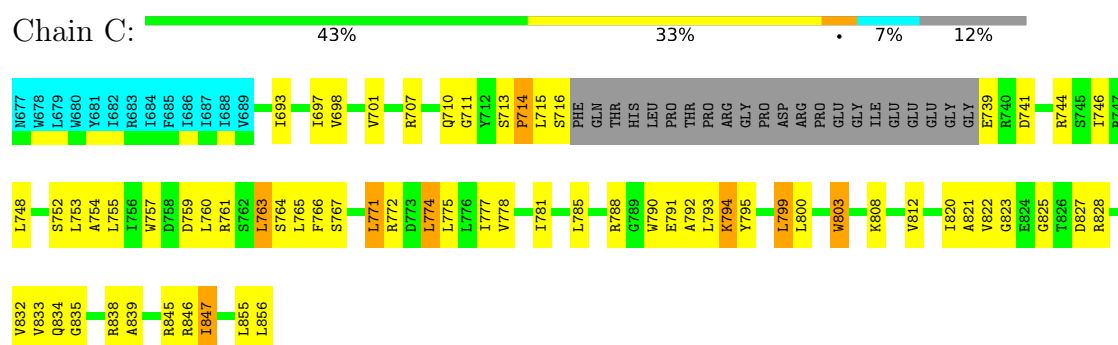
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

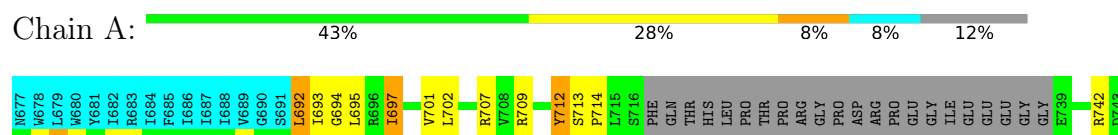


- Molecule 1: Transmembrane protein gp41

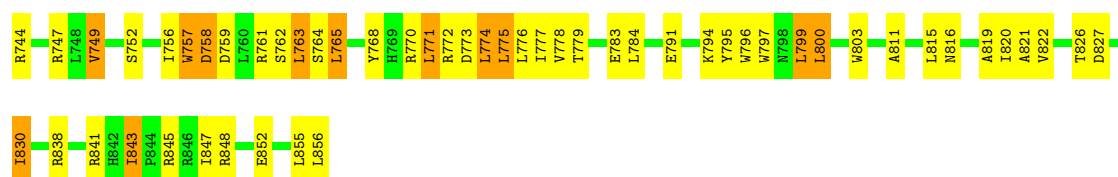


#### 4.2.14 Score per residue for model 14

- Molecule 1: Transmembrane protein gp41

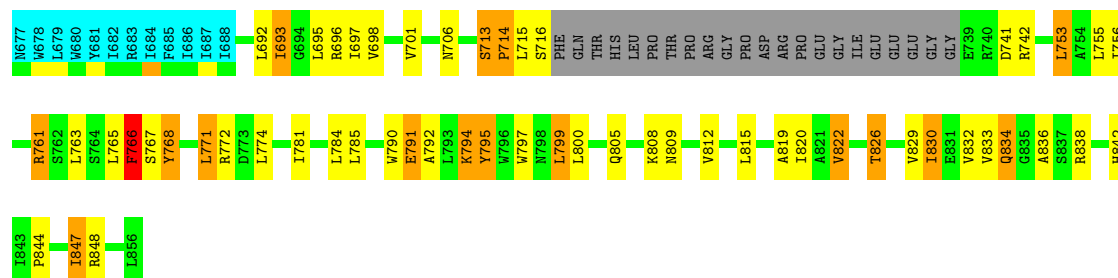






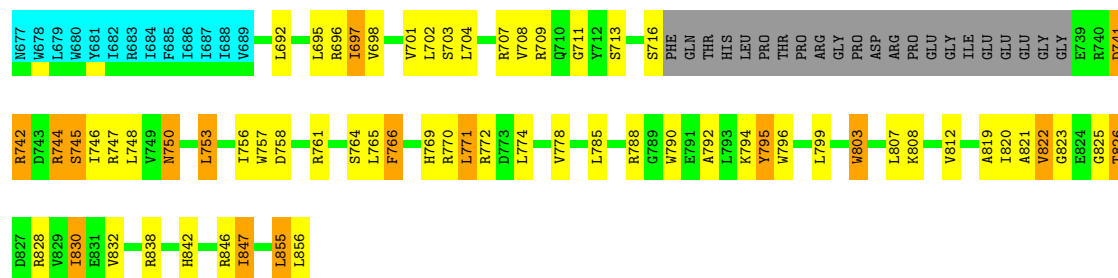
- Molecule 1: Transmembrane protein gp41

Chain B: 49% 22% 9% 7% 12%



- Molecule 1: Transmembrane protein gp41

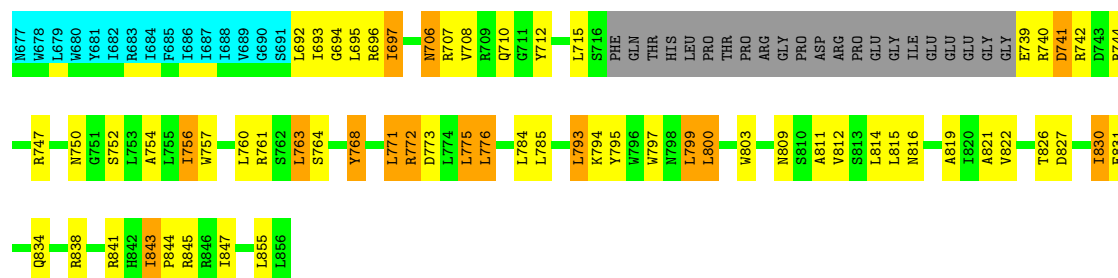
Chain C: 44% 27% 9% 7% 12%



#### 4.2.15 Score per residue for model 15

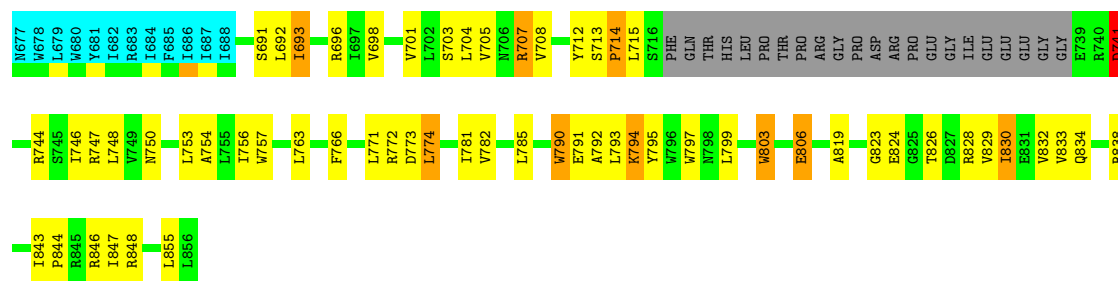
- Molecule 1: Transmembrane protein gp41

Chain A: 44% 27% 8% 8% 12%



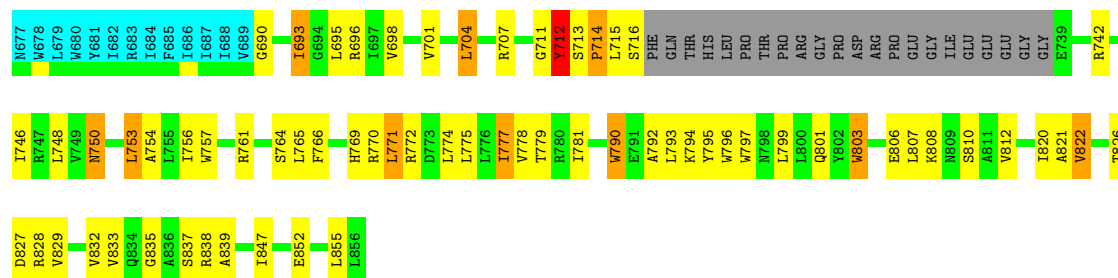
- Molecule 1: Transmembrane protein gp41

Chain B: 47% 28% 5% 7% 12%



• Molecule 1: Transmembrane protein gp41

Chain C: 43% 31% 6% • 7% 12%



## 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	596
Number of shifts mapped to atoms	596
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	0.81±0.01	0±0/1189 ( 0.0± 0.0%)	0.96±0.02	0±1/1606 ( 0.0± 0.1%)
1	B	0.79±0.01	0±0/1206 ( 0.0± 0.0%)	0.96±0.01	0±0/1629 ( 0.0± 0.0%)
1	C	0.80±0.01	0±0/1199 ( 0.0± 0.0%)	0.97±0.01	0±0/1619 ( 0.0± 0.0%)
All	All	0.80	0/53910 ( 0.0%)	0.96	10/72810 ( 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±0.3
1	C	0.0±0.0	0.1±0.2
All	All	0	3

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	-6.37	117.18	121.00	13	1
1	C	742	ARG	NE-CZ-NH2	5.65	123.12	120.30	14	1
1	A	712	TYR	CB-CG-CD1	-5.58	117.65	121.00	9	1
1	B	768	TYR	CB-CG-CD2	-5.30	117.82	121.00	13	1
1	C	795	TYR	CB-CG-CD1	-5.27	117.84	121.00	1	1
1	A	795	TYR	CB-CG-CD2	5.18	124.11	121.00	13	1
1	A	747	ARG	NE-CZ-NH2	5.11	122.85	120.30	13	1
1	B	747	ARG	NE-CZ-NH2	5.06	122.83	120.30	9	1
1	A	797	TRP	CB-CG-CD2	5.04	133.16	126.60	13	1
1	C	795	TYR	CB-CG-CD2	-5.01	117.99	121.00	6	1

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	C	761	ARG	Sidechain	1
1	B	761	ARG	Sidechain	1
1	B	707	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	1171	1235	1232	48±8
1	B	1188	1252	1249	42±8
1	C	1181	1243	1240	42±5
All	All	53100	55950	55815	1674

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:754:ALA:HB1	1:B:715:LEU:HD12	0.89	1.41	1	1
1:A:692:LEU:HD12	1:A:693:ILE:N	0.82	1.90	12	4
1:A:692:LEU:HD23	1:A:696:ARG:CZ	0.80	2.06	13	1
1:B:771:LEU:HD22	1:B:772:ARG:N	0.78	1.93	7	5
1:A:756:ILE:HD13	1:C:795:TYR:CZ	0.78	2.13	13	1
1:B:695:LEU:HD22	1:B:696:ARG:NH1	0.78	1.94	4	3
1:B:698:VAL:O	1:B:701:VAL:HG22	0.76	1.79	15	15
1:A:693:ILE:HD13	1:B:696:ARG:NH1	0.76	1.96	11	1
1:A:771:LEU:HD22	1:A:772:ARG:N	0.75	1.95	8	3
1:A:698:VAL:O	1:A:701:VAL:HG22	0.75	1.82	6	4
1:B:785:LEU:HD23	1:C:750:ASN:ND2	0.75	1.97	7	11
1:B:713:SER:O	1:B:714:PRO:O	0.74	2.04	1	10
1:A:747:ARG:NE	1:C:785:LEU:HD23	0.74	1.98	10	1
1:A:795:TYR:CD2	1:B:756:ILE:HG21	0.74	2.18	8	2
1:A:785:LEU:HD23	1:B:750:ASN:ND2	0.73	1.98	11	8
1:C:698:VAL:O	1:C:701:VAL:HG22	0.73	1.83	4	15
1:C:764:SER:OG	1:C:771:LEU:HD12	0.73	1.83	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:771:LEU:HD13	1:B:772:ARG:N	0.73	1.98	9	3
1:B:704:LEU:O	1:B:708:VAL:HG23	0.72	1.83	3	11
1:A:795:TYR:CG	1:B:756:ILE:HG21	0.72	2.19	3	1
1:B:774:LEU:O	1:B:778:VAL:HG23	0.72	1.83	8	6
1:C:763:LEU:O	1:C:774:LEU:HD13	0.72	1.85	1	3
1:A:847:ILE:HD12	1:A:848:ARG:N	0.72	2.00	14	2
1:B:799:LEU:HD13	1:B:800:LEU:N	0.72	2.00	12	6
1:B:819:ALA:HB1	1:B:826:THR:HG23	0.71	1.61	2	1
1:A:816:ASN:O	1:A:820:ILE:HD12	0.71	1.84	5	7
1:A:793:LEU:HD11	1:A:847:ILE:CD1	0.70	2.16	1	4
1:A:763:LEU:HD22	1:A:764:SER:N	0.70	2.01	15	8
1:C:819:ALA:HB1	1:C:826:THR:CG2	0.69	2.18	8	5
1:B:781:ILE:CG2	1:C:746:ILE:HG21	0.69	2.17	13	2
1:A:763:LEU:O	1:A:774:LEU:HD13	0.69	1.86	1	5
1:A:755:LEU:O	1:A:755:LEU:HD23	0.69	1.87	12	4
1:B:693:ILE:HD13	1:B:693:ILE:O	0.69	1.88	9	5
1:A:793:LEU:HD22	1:A:847:ILE:HD11	0.69	1.63	8	1
1:B:797:TRP:CD1	1:B:847:ILE:HG21	0.69	2.23	14	9
1:B:795:TYR:CB	1:C:756:ILE:HG21	0.69	2.18	2	1
1:A:808:LYS:O	1:A:812:VAL:HG23	0.68	1.87	12	6
1:C:748:LEU:HD13	1:C:748:LEU:O	0.68	1.88	8	4
1:A:693:ILE:HD13	1:B:696:ARG:NH2	0.68	2.02	5	1
1:B:753:LEU:O	1:B:756:ILE:HG22	0.68	1.89	3	5
1:C:777:ILE:HD13	1:C:778:VAL:N	0.67	2.03	2	1
1:A:812:VAL:HG22	1:A:834:GLN:OE1	0.67	1.89	6	2
1:C:812:VAL:HG12	1:C:834:GLN:NE2	0.67	2.05	8	1
1:A:742:ARG:CZ	1:A:746:ILE:HD11	0.67	2.19	13	1
1:C:704:LEU:HD22	1:C:707:ARG:NH2	0.67	2.04	15	1
1:B:799:LEU:CD1	1:B:800:LEU:HD22	0.67	2.19	3	1
1:A:692:LEU:HD13	1:A:693:ILE:N	0.67	2.03	10	2
1:B:764:SER:OG	1:B:771:LEU:HD12	0.67	1.88	13	2
1:C:774:LEU:HD13	1:C:777:ILE:CG1	0.67	2.20	13	1
1:A:799:LEU:CD2	1:B:760:LEU:HD13	0.66	2.20	5	2
1:A:795:TYR:CD1	1:B:756:ILE:HG21	0.66	2.25	3	1
1:A:764:SER:CB	1:A:771:LEU:HD12	0.66	2.20	11	4
1:B:715:LEU:O	1:B:715:LEU:HD23	0.66	1.90	12	2
1:A:819:ALA:HB1	1:A:826:THR:CG2	0.66	2.21	14	3
1:A:816:ASN:OD1	1:A:830:ILE:HD11	0.66	1.89	6	5
1:A:755:LEU:HG	1:B:715:LEU:HD21	0.66	1.68	12	1
1:C:763:LEU:HD22	1:C:764:SER:N	0.66	2.06	13	1
1:A:759:ASP:OD2	1:A:763:LEU:HD11	0.66	1.89	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:793:LEU:HD12	1:A:847:ILE:HD11	0.66	1.65	6	3
1:C:697:ILE:HD13	1:C:697:ILE:O	0.66	1.90	8	8
1:B:777:ILE:HD12	1:B:778:VAL:N	0.66	2.06	7	3
1:A:785:LEU:HD21	1:B:747:ARG:HG2	0.66	1.66	9	2
1:A:795:TYR:CE2	1:B:756:ILE:HG21	0.66	2.26	8	1
1:A:764:SER:OG	1:A:771:LEU:HD12	0.66	1.91	15	2
1:B:781:ILE:HD12	1:B:782:VAL:N	0.66	2.05	15	1
1:A:774:LEU:HD23	1:A:775:LEU:N	0.65	2.05	10	3
1:B:697:ILE:O	1:B:697:ILE:HD13	0.65	1.91	2	1
1:C:778:VAL:O	1:C:781:ILE:HG22	0.65	1.91	6	2
1:C:774:LEU:HD23	1:C:777:ILE:HG12	0.65	1.66	11	2
1:B:693:ILE:HD11	1:C:696:ARG:NE	0.65	2.05	1	3
1:C:694:GLY:O	1:C:697:ILE:HG22	0.65	1.92	10	5
1:B:756:ILE:HD13	1:B:756:ILE:O	0.65	1.91	3	5
1:A:793:LEU:HD11	1:A:847:ILE:HG13	0.65	1.69	9	2
1:A:821:ALA:O	1:A:822:VAL:HG13	0.65	1.91	1	4
1:B:791:GLU:O	1:B:794:LYS:HG3	0.64	1.92	3	14
1:B:819:ALA:HB1	1:B:826:THR:CG2	0.64	2.22	2	2
1:B:715:LEU:HD13	1:B:715:LEU:O	0.64	1.92	1	1
1:A:819:ALA:HB1	1:A:826:THR:HB	0.64	1.69	8	7
1:A:771:LEU:HD12	1:A:771:LEU:C	0.64	2.11	13	2
1:C:775:LEU:O	1:C:778:VAL:HG22	0.64	1.92	7	9
1:C:764:SER:CB	1:C:771:LEU:HD12	0.64	2.22	7	4
1:B:693:ILE:HD11	1:C:696:ARG:HG3	0.64	1.68	9	4
1:B:781:ILE:HG21	1:C:746:ILE:HG21	0.64	1.69	13	1
1:B:693:ILE:HD12	1:C:696:ARG:HG3	0.63	1.70	6	3
1:C:710:GLN:O	1:C:715:LEU:HD12	0.63	1.93	5	1
1:A:791:GLU:CB	1:B:753:LEU:HD22	0.63	2.24	11	3
1:C:806:GLU:CG	1:C:807:LEU:HD22	0.63	2.23	7	1
1:B:693:ILE:HD11	1:C:696:ARG:CG	0.63	2.24	9	3
1:A:800:LEU:HD22	1:A:803:TRP:CZ3	0.63	2.29	12	12
1:B:781:ILE:HG23	1:C:746:ILE:HG21	0.63	1.71	9	2
1:A:812:VAL:HG21	1:A:834:GLN:OE1	0.63	1.93	1	2
1:A:777:ILE:HD13	1:B:743:ASP:OD2	0.63	1.94	9	1
1:C:781:ILE:CD1	1:C:785:LEU:HD13	0.62	2.24	8	1
1:A:796:TRP:HE1	1:B:756:ILE:HD12	0.62	1.54	12	2
1:C:819:ALA:HB1	1:C:826:THR:HG21	0.62	1.70	3	1
1:A:697:ILE:O	1:A:697:ILE:HD13	0.62	1.94	1	9
1:A:793:LEU:O	1:A:793:LEU:HD13	0.62	1.92	11	3
1:C:704:LEU:HD13	1:C:707:ARG:CZ	0.62	2.24	3	1
1:C:764:SER:O	1:C:765:LEU:HD23	0.62	1.94	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:759:ASP:O	1:A:763:LEU:HD12	0.62	1.95	11	3
1:A:742:ARG:NH2	1:A:746:ILE:HD11	0.62	2.09	13	1
1:A:748:LEU:HD21	1:B:714:PRO:HG2	0.62	1.71	1	1
1:A:746:ILE:HG12	1:C:781:ILE:HD12	0.62	1.70	11	3
1:C:771:LEU:HA	1:C:774:LEU:HD12	0.62	1.71	11	1
1:A:768:TYR:CZ	1:A:771:LEU:HD23	0.62	2.30	13	1
1:C:806:GLU:HG3	1:C:807:LEU:HD22	0.62	1.69	7	2
1:B:790:TRP:CZ2	1:B:793:LEU:HD13	0.61	2.30	1	3
1:C:756:ILE:O	1:C:756:ILE:HD13	0.61	1.93	5	1
1:A:692:LEU:HD23	1:C:693:ILE:HG21	0.61	1.71	9	1
1:A:800:LEU:HD22	1:A:803:TRP:CH2	0.61	2.30	13	5
1:B:774:LEU:CD2	1:B:777:ILE:HD11	0.61	2.24	9	2
1:A:764:SER:HB3	1:A:771:LEU:HD12	0.61	1.72	4	5
1:B:774:LEU:HD12	1:B:775:LEU:N	0.61	2.10	10	1
1:A:715:LEU:HB3	1:C:754:ALA:HB1	0.61	1.72	11	3
1:C:762:SER:O	1:C:774:LEU:HD22	0.61	1.96	6	2
1:A:715:LEU:HD21	1:C:758:ASP:CG	0.61	2.16	2	1
1:A:745:SER:O	1:A:749:VAL:HG23	0.61	1.95	12	1
1:A:746:ILE:HG21	1:C:781:ILE:HG23	0.61	1.72	1	1
1:A:763:LEU:HD13	1:A:764:SER:H	0.61	1.55	10	3
1:B:756:ILE:HG23	1:B:757:TRP:CE3	0.61	2.30	8	1
1:A:704:LEU:HD21	1:B:707:ARG:HG2	0.61	1.73	12	1
1:A:819:ALA:HB1	1:A:826:THR:HG22	0.61	1.72	12	2
1:A:816:ASN:HD22	1:A:830:ILE:HD11	0.60	1.56	3	1
1:B:763:LEU:HD23	1:B:764:SER:H	0.60	1.55	10	1
1:B:694:GLY:O	1:B:697:ILE:HG22	0.60	1.96	2	1
1:B:795:TYR:CG	1:C:756:ILE:HG21	0.60	2.30	2	1
1:C:753:LEU:O	1:C:756:ILE:HG22	0.60	1.96	2	5
1:C:774:LEU:HD23	1:C:777:ILE:CG1	0.60	2.26	4	2
1:A:799:LEU:HB3	1:A:803:TRP:CH2	0.60	2.31	14	5
1:B:705:VAL:HG21	1:B:748:LEU:HD22	0.60	1.72	8	2
1:C:819:ALA:HB1	1:C:826:THR:HG22	0.60	1.74	8	2
1:B:774:LEU:HD13	1:B:774:LEU:O	0.60	1.97	4	4
1:A:755:LEU:HB2	1:B:715:LEU:HD22	0.59	1.75	4	1
1:A:816:ASN:O	1:A:820:ILE:HD13	0.59	1.96	14	2
1:C:826:THR:O	1:C:830:ILE:HG22	0.59	1.98	1	2
1:C:820:ILE:O	1:C:822:VAL:HG12	0.59	1.97	5	2
1:A:781:ILE:CG1	1:B:746:ILE:HG21	0.59	2.27	7	1
1:B:791:GLU:CD	1:C:753:LEU:HD22	0.59	2.18	8	1
1:C:765:LEU:HD13	1:C:774:LEU:HD21	0.59	1.74	11	1
1:A:791:GLU:HB2	1:B:753:LEU:HD22	0.59	1.73	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:713:SER:O	1:A:714:PRO:O	0.59	2.20	13	3
1:C:792:ALA:HA	1:C:795:TYR:CZ	0.59	2.33	7	3
1:C:748:LEU:HD22	1:C:748:LEU:O	0.59	1.98	1	1
1:A:755:LEU:HD12	1:B:715:LEU:HD11	0.59	1.75	11	1
1:A:811:ALA:HB1	1:A:815:LEU:CD1	0.59	2.27	5	4
1:C:755:LEU:HD23	1:C:755:LEU:O	0.59	1.97	7	1
1:A:750:ASN:OD1	1:C:785:LEU:HD23	0.58	1.97	2	1
1:A:793:LEU:HD11	1:A:847:ILE:HD11	0.58	1.75	4	3
1:A:799:LEU:HD11	1:B:756:ILE:HG21	0.58	1.73	4	1
1:B:774:LEU:O	1:B:774:LEU:HD13	0.58	1.97	8	1
1:A:819:ALA:HB1	1:A:826:THR:CB	0.58	2.29	7	1
1:B:695:LEU:HD23	1:B:695:LEU:O	0.58	1.99	3	6
1:B:819:ALA:HB1	1:B:826:THR:OG1	0.58	1.97	13	4
1:A:713:SER:HB2	1:C:708:VAL:HG23	0.58	1.73	12	1
1:A:816:ASN:CG	1:A:830:ILE:HD11	0.58	2.18	7	4
1:B:785:LEU:HD21	1:C:747:ARG:HG2	0.58	1.76	7	1
1:C:799:LEU:O	1:C:803:TRP:CE3	0.58	2.57	2	8
1:A:812:VAL:HG22	1:A:834:GLN:HG3	0.58	1.74	12	2
1:A:696:ARG:HE	1:C:693:ILE:HD11	0.58	1.59	15	6
1:A:756:ILE:HD13	1:C:795:TYR:CE1	0.58	2.34	13	1
1:A:754:ALA:HB1	1:B:715:LEU:HB3	0.57	1.75	2	2
1:A:793:LEU:HD12	1:A:847:ILE:CD1	0.57	2.29	6	1
1:C:710:GLN:O	1:C:715:LEU:HD13	0.57	1.99	13	1
1:A:748:LEU:HD21	1:B:714:PRO:CG	0.57	2.29	1	1
1:B:771:LEU:H	1:B:771:LEU:HD13	0.57	1.58	1	3
1:B:771:LEU:HD13	1:B:772:ARG:H	0.57	1.57	12	3
1:C:693:ILE:HD12	1:C:693:ILE:O	0.57	2.00	11	4
1:A:763:LEU:HD13	1:A:764:SER:N	0.57	2.15	10	3
1:A:763:LEU:HD22	1:A:763:LEU:C	0.57	2.20	11	10
1:A:781:ILE:HG23	1:B:746:ILE:HG12	0.57	1.76	13	1
1:A:793:LEU:C	1:A:793:LEU:HD13	0.57	2.19	9	6
1:B:819:ALA:HB1	1:B:826:THR:HB	0.57	1.75	10	4
1:C:830:ILE:HD13	1:C:830:ILE:O	0.57	1.99	9	2
1:C:742:ARG:O	1:C:746:ILE:HD12	0.57	2.00	12	1
1:B:774:LEU:HD22	1:B:777:ILE:HD11	0.57	1.76	12	4
1:A:812:VAL:HG22	1:A:834:GLN:CD	0.57	2.20	6	1
1:A:821:ALA:O	1:A:822:VAL:HG22	0.57	1.99	5	1
1:B:760:LEU:C	1:B:760:LEU:HD23	0.57	2.20	13	5
1:A:775:LEU:HD23	1:A:776:LEU:N	0.57	2.15	12	9
1:C:774:LEU:O	1:C:777:ILE:HG13	0.57	2.00	10	1
1:C:765:LEU:HB2	1:C:774:LEU:HD21	0.56	1.77	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:715:LEU:HD11	1:C:739:GLU:OE1	0.56	2.00	5	1
1:A:855:LEU:C	1:A:856:LEU:HD23	0.56	2.21	5	3
1:B:774:LEU:HD21	1:C:742:ARG:CZ	0.56	2.30	9	1
1:C:790:TRP:CZ2	1:C:793:LEU:HD13	0.56	2.35	13	1
1:B:781:ILE:HD13	1:C:746:ILE:HG21	0.56	1.76	15	1
1:A:771:LEU:HD12	1:A:772:ARG:N	0.56	2.15	1	3
1:A:763:LEU:O	1:A:774:LEU:HD22	0.56	2.00	2	1
1:C:820:ILE:O	1:C:822:VAL:N	0.56	2.38	9	8
1:B:765:LEU:HD12	1:B:774:LEU:HD23	0.56	1.76	9	1
1:B:797:TRP:NE1	1:B:847:ILE:HG21	0.56	2.16	10	1
1:A:692:LEU:HD13	1:C:693:ILE:HG12	0.56	1.77	12	1
1:C:829:VAL:O	1:C:833:VAL:HG22	0.56	1.99	7	8
1:A:754:ALA:HB3	1:B:715:LEU:O	0.56	2.00	15	2
1:C:771:LEU:H	1:C:771:LEU:HD13	0.56	1.59	4	8
1:A:793:LEU:O	1:A:793:LEU:HD23	0.56	2.00	8	1
1:A:799:LEU:HD23	1:A:803:TRP:CZ2	0.56	2.36	15	3
1:C:771:LEU:HD22	1:C:771:LEU:N	0.56	2.15	10	11
1:A:777:ILE:HD12	1:A:778:VAL:N	0.56	2.15	9	3
1:A:713:SER:CB	1:C:708:VAL:HG23	0.56	2.30	12	1
1:B:791:GLU:HB2	1:C:753:LEU:HD22	0.55	1.78	1	1
1:A:708:VAL:HG21	1:B:714:PRO:HD2	0.55	1.77	7	2
1:A:785:LEU:CD2	1:B:749:VAL:HG13	0.55	2.31	13	1
1:A:795:TYR:O	1:A:799:LEU:HD12	0.55	2.02	4	2
1:A:763:LEU:HD12	1:A:763:LEU:H	0.55	1.61	7	1
1:A:747:ARG:HE	1:C:785:LEU:HD23	0.55	1.59	10	1
1:A:763:LEU:N	1:A:763:LEU:HD13	0.55	2.16	14	1
1:B:830:ILE:HD13	1:B:830:ILE:O	0.55	2.02	3	9
1:A:802:TYR:OH	1:B:760:LEU:HD21	0.55	2.00	2	2
1:C:764:SER:O	1:C:765:LEU:HB2	0.55	2.02	5	1
1:A:796:TRP:NE1	1:B:756:ILE:HD12	0.55	2.17	14	2
1:C:748:LEU:HD13	1:C:749:VAL:N	0.55	2.16	1	1
1:C:765:LEU:HB2	1:C:774:LEU:HD11	0.55	1.77	11	3
1:A:781:ILE:HD12	1:B:746:ILE:HG12	0.55	1.77	13	2
1:A:820:ILE:O	1:A:822:VAL:N	0.55	2.40	1	3
1:B:774:LEU:HD13	1:B:777:ILE:HD11	0.55	1.78	1	2
1:C:840:ILE:HD13	1:C:840:ILE:O	0.55	2.01	2	1
1:A:764:SER:O	1:A:770:ARG:HB2	0.55	2.01	14	3
1:A:756:ILE:HG23	1:C:795:TYR:HB2	0.55	1.78	9	3
1:A:795:TYR:HB3	1:B:756:ILE:HG21	0.55	1.79	9	1
1:C:777:ILE:HD12	1:C:778:VAL:N	0.55	2.17	10	2
1:B:704:LEU:HD11	1:C:712:TYR:CD2	0.55	2.37	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:771:LEU:H	1:A:771:LEU:HD13	0.54	1.62	2	7
1:B:808:LYS:O	1:B:812:VAL:HG22	0.54	2.02	1	1
1:C:792:ALA:O	1:C:795:TYR:CD2	0.54	2.61	10	5
1:A:709:ARG:CZ	1:C:761:ARG:CZ	0.54	2.85	9	1
1:A:749:VAL:HG21	1:C:781:ILE:HD11	0.54	1.79	9	1
1:B:797:TRP:CE2	1:B:847:ILE:HD13	0.54	2.38	14	3
1:A:693:ILE:HD12	1:A:694:GLY:N	0.54	2.18	15	6
1:A:785:LEU:HD13	1:B:750:ASN:CG	0.54	2.22	13	1
1:A:754:ALA:HB1	1:B:715:LEU:CD1	0.54	2.25	1	1
1:C:768:TYR:CD2	1:C:771:LEU:HD11	0.54	2.37	3	1
1:B:753:LEU:HD12	1:B:754:ALA:N	0.54	2.18	12	6
1:C:695:LEU:HD22	1:C:696:ARG:HH22	0.54	1.63	15	2
1:C:808:LYS:O	1:C:812:VAL:HG13	0.54	2.02	8	1
1:A:820:ILE:HD11	1:A:827:ASP:CA	0.54	2.33	14	1
1:B:704:LEU:HD22	1:C:712:TYR:CB	0.54	2.32	6	1
1:A:705:VAL:HG13	1:A:748:LEU:CD2	0.54	2.33	7	1
1:A:753:LEU:HA	1:C:795:TYR:CD1	0.54	2.37	7	1
1:A:826:THR:O	1:A:829:VAL:HG22	0.54	2.03	3	8
1:B:697:ILE:HD12	1:B:698:VAL:N	0.54	2.17	3	5
1:A:795:TYR:C	1:A:799:LEU:HD12	0.54	2.23	4	1
1:A:811:ALA:HB1	1:A:815:LEU:HD12	0.54	1.78	5	3
1:A:815:LEU:HB2	1:A:830:ILE:HD13	0.54	1.80	5	1
1:A:843:ILE:H	1:A:843:ILE:HD13	0.54	1.62	2	12
1:A:692:LEU:HD22	1:A:692:LEU:C	0.54	2.22	13	2
1:A:693:ILE:HG22	1:C:693:ILE:HG21	0.54	1.80	13	1
1:C:760:LEU:O	1:C:760:LEU:HD23	0.53	2.03	7	1
1:B:774:LEU:HD12	1:B:775:LEU:H	0.53	1.62	10	1
1:B:778:VAL:O	1:B:781:ILE:HG22	0.53	2.03	2	2
1:B:751:GLY:O	1:B:754:ALA:HB3	0.53	2.03	7	1
1:A:812:VAL:HG21	1:A:834:GLN:CG	0.53	2.33	10	1
1:A:768:TYR:OH	1:A:771:LEU:HD23	0.53	2.03	13	1
1:A:742:ARG:NH2	1:C:774:LEU:HD12	0.53	2.18	2	1
1:C:753:LEU:HD12	1:C:754:ALA:N	0.53	2.18	2	1
1:A:695:LEU:O	1:A:698:VAL:HG12	0.53	2.04	2	7
1:A:715:LEU:O	1:C:754:ALA:HB3	0.53	2.04	1	1
1:B:693:ILE:HD11	1:C:696:ARG:HE	0.53	1.63	1	1
1:C:797:TRP:CD1	1:C:847:ILE:HD11	0.53	2.38	15	3
1:B:791:GLU:OE1	1:C:753:LEU:HD22	0.53	2.04	8	1
1:B:803:TRP:N	1:B:803:TRP:CE3	0.53	2.76	12	14
1:B:795:TYR:HB3	1:C:756:ILE:HG21	0.53	1.81	2	1
1:B:803:TRP:N	1:B:803:TRP:HE3	0.53	2.01	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:756:ILE:HD12	1:C:795:TYR:O	0.53	2.03	6	1
1:A:819:ALA:HB1	1:A:826:THR:HG21	0.53	1.79	15	1
1:A:747:ARG:HA	1:C:785:LEU:HD23	0.53	1.80	1	1
1:B:785:LEU:HD23	1:C:750:ASN:HD21	0.53	1.64	7	2
1:C:803:TRP:N	1:C:803:TRP:CE3	0.52	2.76	8	8
1:B:695:LEU:HD22	1:B:696:ARG:HH11	0.52	1.63	3	1
1:C:830:ILE:HG23	1:C:831:GLU:OE1	0.52	2.04	1	1
1:C:795:TYR:O	1:C:799:LEU:HB2	0.52	2.04	8	2
1:C:763:LEU:HD23	1:C:764:SER:N	0.52	2.18	1	2
1:A:799:LEU:HD21	1:B:760:LEU:HD13	0.52	1.80	5	1
1:A:702:LEU:O	1:A:705:VAL:HG23	0.52	2.04	11	1
1:C:756:ILE:C	1:C:756:ILE:HD13	0.52	2.25	2	1
1:A:774:LEU:O	1:A:778:VAL:HG23	0.52	2.05	12	6
1:C:765:LEU:CB	1:C:774:LEU:HD21	0.52	2.34	13	1
1:A:768:TYR:CD2	1:C:803:TRP:CD2	0.52	2.98	1	1
1:A:692:LEU:HD21	1:C:693:ILE:CD1	0.52	2.35	10	2
1:B:829:VAL:O	1:B:833:VAL:HG12	0.52	2.05	9	11
1:B:704:LEU:HD22	1:C:712:TYR:HB3	0.52	1.82	6	1
1:B:829:VAL:O	1:B:833:VAL:HG23	0.52	2.05	8	1
1:C:774:LEU:O	1:C:778:VAL:HG13	0.52	2.04	14	1
1:B:705:VAL:CG2	1:B:748:LEU:HD22	0.52	2.35	8	1
1:B:754:ALA:HB1	1:C:715:LEU:O	0.52	2.05	3	3
1:A:760:LEU:O	1:A:763:LEU:HD13	0.51	2.06	8	2
1:A:785:LEU:HD23	1:B:750:ASN:CG	0.51	2.26	6	3
1:B:794:LYS:HD3	1:B:795:TYR:N	0.51	2.20	2	1
1:A:816:ASN:ND2	1:A:830:ILE:HD11	0.51	2.20	13	2
1:A:751:GLY:O	1:A:754:ALA:HB3	0.51	2.04	12	1
1:A:771:LEU:C	1:A:771:LEU:CD1	0.51	2.79	13	2
1:A:816:ASN:HB2	1:A:830:ILE:HD11	0.51	1.82	8	2
1:A:830:ILE:C	1:A:830:ILE:HD12	0.51	2.26	13	13
1:A:781:ILE:HB	1:B:746:ILE:HG21	0.51	1.81	2	1
1:C:756:ILE:HD13	1:C:756:ILE:O	0.51	2.05	2	1
1:C:760:LEU:HD21	1:C:768:TYR:OH	0.51	2.05	5	1
1:A:709:ARG:O	1:C:761:ARG:NH1	0.51	2.43	8	1
1:A:768:TYR:CE2	1:A:771:LEU:HD23	0.51	2.40	1	1
1:C:745:SER:O	1:C:748:LEU:HD23	0.51	2.05	3	1
1:B:754:ALA:HB1	1:C:715:LEU:HB3	0.51	1.82	7	1
1:C:765:LEU:HD13	1:C:774:LEU:HD11	0.51	1.83	2	1
1:B:794:LYS:HD2	1:C:753:LEU:HD13	0.51	1.82	3	1
1:A:704:LEU:HD12	1:B:712:TYR:O	0.51	2.06	6	1
1:C:797:TRP:NE1	1:C:847:ILE:HD11	0.51	2.21	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:793:LEU:HD11	1:A:847:ILE:CG1	0.51	2.35	4	3
1:A:748:LEU:HD23	1:B:714:PRO:CG	0.51	2.36	5	2
1:A:697:ILE:HD11	1:B:696:ARG:HD2	0.51	1.82	13	1
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.51	1.82	1	2
1:A:694:GLY:O	1:A:697:ILE:HG22	0.51	2.06	1	5
1:A:760:LEU:HD13	1:C:799:LEU:HD11	0.51	1.82	1	2
1:A:760:LEU:HD23	1:A:760:LEU:O	0.51	2.05	12	3
1:C:771:LEU:HD22	1:C:771:LEU:H	0.51	1.64	3	6
1:A:695:LEU:HD23	1:A:695:LEU:O	0.51	2.06	5	2
1:C:748:LEU:C	1:C:748:LEU:HD13	0.51	2.26	14	4
1:A:706:ASN:OD1	1:C:704:LEU:HD11	0.51	2.05	9	1
1:C:763:LEU:O	1:C:774:LEU:HD22	0.50	2.06	3	1
1:B:765:LEU:CD1	1:B:774:LEU:HD23	0.50	2.37	9	1
1:C:803:TRP:N	1:C:803:TRP:HE3	0.50	2.04	7	11
1:A:710:GLN:OE1	1:C:704:LEU:HD21	0.50	2.06	3	1
1:A:856:LEU:HD12	1:A:856:LEU:O	0.50	2.06	6	1
1:C:778:VAL:O	1:C:782:VAL:HG23	0.50	2.07	10	1
1:C:828:ARG:O	1:C:832:VAL:HG23	0.50	2.05	3	14
1:C:695:LEU:O	1:C:698:VAL:HG12	0.50	2.05	4	4
1:A:746:ILE:CG1	1:C:781:ILE:HG23	0.50	2.37	11	1
1:A:746:ILE:HG21	1:C:781:ILE:HG13	0.50	1.81	3	1
1:A:772:ARG:O	1:A:775:LEU:HD22	0.50	2.05	3	5
1:A:768:TYR:CZ	1:C:803:TRP:CZ3	0.50	2.98	8	1
1:C:815:LEU:HB3	1:C:830:ILE:HD11	0.50	1.84	8	3
1:A:820:ILE:HD11	1:A:827:ASP:HA	0.50	1.83	14	1
1:B:756:ILE:HD13	1:B:756:ILE:C	0.50	2.26	3	2
1:B:799:LEU:O	1:B:803:TRP:CE3	0.50	2.65	8	4
1:B:797:TRP:NE1	1:B:847:ILE:HD13	0.50	2.21	9	2
1:A:800:LEU:HD22	1:A:803:TRP:HZ3	0.50	1.65	14	3
1:C:830:ILE:HG23	1:C:831:GLU:CD	0.50	2.27	1	1
1:A:755:LEU:HD12	1:B:715:LEU:CD1	0.50	2.37	3	1
1:B:806:GLU:HB3	1:C:771:LEU:HD21	0.50	1.84	7	3
1:C:847:ILE:H	1:C:847:ILE:HD13	0.50	1.66	13	5
1:C:756:ILE:CD1	1:C:760:LEU:HD12	0.50	2.37	7	1
1:A:797:TRP:CG	1:A:847:ILE:HD11	0.50	2.42	9	1
1:C:795:TYR:CZ	1:C:796:TRP:NE1	0.50	2.79	14	2
1:A:693:ILE:HD12	1:A:693:ILE:O	0.50	2.06	8	1
1:C:761:ARG:O	1:C:765:LEU:HD12	0.50	2.07	8	1
1:A:753:LEU:HD22	1:C:791:GLU:OE2	0.50	2.07	12	1
1:A:763:LEU:HD13	1:A:763:LEU:H	0.50	1.67	14	1
1:B:795:TYR:CG	1:C:756:ILE:HB	0.50	2.42	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:713:SER:O	1:A:714:PRO:C	0.49	2.51	2	7
1:C:771:LEU:HD23	1:C:772:ARG:HD3	0.49	1.83	2	2
1:B:693:ILE:HD11	1:C:696:ARG:CD	0.49	2.37	4	3
1:A:696:ARG:NE	1:C:693:ILE:HD11	0.49	2.21	15	5
1:B:795:TYR:O	1:C:756:ILE:HD12	0.49	2.06	9	1
1:A:747:ARG:CZ	1:A:750:ASN:CG	0.49	2.80	10	1
1:C:781:ILE:HG22	1:C:785:LEU:HD22	0.49	1.84	13	1
1:A:756:ILE:CD1	1:C:799:LEU:HD13	0.49	2.37	1	1
1:B:758:ASP:HB3	1:C:715:LEU:HD13	0.49	1.83	5	1
1:B:759:ASP:O	1:B:763:LEU:HD22	0.49	2.06	10	1
1:C:763:LEU:HD23	1:C:763:LEU:C	0.49	2.27	9	8
1:A:792:ALA:HA	1:A:795:TYR:CE1	0.49	2.42	7	1
1:A:800:LEU:C	1:A:800:LEU:HD13	0.49	2.28	8	1
1:A:693:ILE:HD13	1:B:696:ARG:CZ	0.49	2.37	11	1
1:B:704:LEU:HD13	1:B:707:ARG:CZ	0.49	2.37	8	1
1:A:755:LEU:HD12	1:B:715:LEU:HD13	0.49	1.84	3	1
1:B:693:ILE:C	1:B:693:ILE:HD13	0.49	2.28	5	3
1:A:775:LEU:O	1:A:778:VAL:HG12	0.49	2.07	8	1
1:B:771:LEU:HD22	1:B:771:LEU:C	0.49	2.28	8	2
1:B:746:ILE:O	1:B:749:VAL:HG12	0.49	2.07	13	1
1:C:760:LEU:HD23	1:C:761:ARG:N	0.49	2.22	1	1
1:B:705:VAL:HG13	1:B:745:SER:HB3	0.49	1.85	2	1
1:A:799:LEU:CD1	1:B:756:ILE:HG21	0.49	2.37	4	2
1:C:808:LYS:O	1:C:812:VAL:HG12	0.49	2.07	13	10
1:A:695:LEU:HD22	1:A:696:ARG:HH22	0.49	1.68	12	1
1:A:756:ILE:HG21	1:C:795:TYR:CD2	0.49	2.42	8	1
1:A:768:TYR:CD2	1:A:771:LEU:HD11	0.49	2.43	11	1
1:B:693:ILE:C	1:B:693:ILE:HD12	0.49	2.28	11	1
1:B:826:THR:O	1:B:829:VAL:HG12	0.49	2.08	14	2
1:C:790:TRP:C	1:C:792:ALA:N	0.49	2.66	9	13
1:A:704:LEU:HD13	1:A:707:ARG:NH2	0.48	2.23	7	1
1:A:799:LEU:HG	1:A:803:TRP:CZ2	0.48	2.43	7	1
1:B:781:ILE:HD13	1:C:743:ASP:O	0.48	2.07	9	1
1:A:693:ILE:HD13	1:B:696:ARG:CG	0.48	2.38	12	1
1:B:781:ILE:HD12	1:B:782:VAL:HG23	0.48	1.85	15	1
1:A:753:LEU:HD13	1:C:791:GLU:CB	0.48	2.38	13	1
1:C:744:ARG:NH2	1:C:745:SER:HA	0.48	2.23	14	1
1:C:792:ALA:O	1:C:795:TYR:CD1	0.48	2.66	6	5
1:A:705:VAL:HG13	1:A:748:LEU:HD23	0.48	1.84	7	1
1:B:795:TYR:CE2	1:B:796:TRP:CD1	0.48	3.01	9	6
1:C:753:LEU:O	1:C:753:LEU:HD12	0.48	2.09	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:695:LEU:HD22	1:C:696:ARG:NH2	0.48	2.22	4	1
1:C:819:ALA:O	1:C:826:THR:HG21	0.48	2.09	6	2
1:A:747:ARG:NE	1:A:750:ASN:ND2	0.48	2.62	10	1
1:C:713:SER:O	1:C:714:PRO:O	0.48	2.30	1	2
1:A:692:LEU:HD13	1:A:693:ILE:H	0.48	1.68	10	2
1:B:792:ALA:HA	1:B:795:TYR:CZ	0.48	2.43	12	1
1:A:793:LEU:CG	1:A:847:ILE:HD11	0.48	2.39	11	1
1:A:704:LEU:HD21	1:B:707:ARG:CG	0.48	2.39	12	1
1:A:704:LEU:CD2	1:B:707:ARG:HG2	0.48	2.39	12	1
1:B:705:VAL:CG2	1:B:748:LEU:HD13	0.48	2.38	1	1
1:A:781:ILE:HD12	1:B:746:ILE:CG1	0.48	2.38	13	2
1:C:748:LEU:HD13	1:C:748:LEU:C	0.48	2.29	6	3
1:C:843:ILE:HG23	1:C:843:ILE:O	0.48	2.08	9	3
1:A:799:LEU:HD11	1:B:756:ILE:CG2	0.48	2.39	4	1
1:A:771:LEU:H	1:A:771:LEU:HD22	0.48	1.68	11	1
1:A:753:LEU:HD12	1:A:754:ALA:N	0.48	2.24	10	5
1:C:756:ILE:HG23	1:C:757:TRP:N	0.48	2.23	14	4
1:A:746:ILE:HG12	1:C:781:ILE:HG23	0.48	1.85	11	1
1:A:768:TYR:CZ	1:C:803:TRP:CE3	0.48	3.01	13	1
1:B:819:ALA:HB1	1:B:826:THR:CB	0.47	2.39	15	5
1:A:756:ILE:HG23	1:C:795:TYR:HD1	0.47	1.68	5	1
1:C:704:LEU:O	1:C:708:VAL:HG23	0.47	2.09	7	1
1:A:799:LEU:HD21	1:B:760:LEU:HD12	0.47	1.86	11	1
1:B:799:LEU:HD13	1:B:799:LEU:C	0.47	2.29	14	1
1:C:774:LEU:HA	1:C:777:ILE:HG23	0.47	1.85	2	1
1:B:774:LEU:C	1:B:774:LEU:HD13	0.47	2.30	9	5
1:A:695:LEU:HD22	1:A:696:ARG:NH2	0.47	2.23	8	3
1:B:768:TYR:CD1	1:B:771:LEU:HD11	0.47	2.44	13	1
1:A:704:LEU:HD21	1:B:707:ARG:HG3	0.47	1.84	3	1
1:C:761:ARG:CZ	1:C:762:SER:HB2	0.47	2.39	4	1
1:C:704:LEU:C	1:C:704:LEU:HD13	0.47	2.28	12	1
1:C:792:ALA:HA	1:C:795:TYR:CE2	0.47	2.44	13	1
1:A:705:VAL:HG22	1:A:748:LEU:HD22	0.47	1.86	2	1
1:B:756:ILE:O	1:B:760:LEU:HB2	0.47	2.09	9	1
1:A:704:LEU:HD21	1:B:707:ARG:CD	0.47	2.40	12	1
1:C:765:LEU:CD1	1:C:774:LEU:HD21	0.47	2.40	12	1
1:B:781:ILE:HG22	1:C:746:ILE:HG21	0.47	1.86	14	1
1:A:756:ILE:HG22	1:C:799:LEU:HD12	0.47	1.85	11	2
1:B:774:LEU:HD23	1:B:774:LEU:O	0.47	2.09	13	1
1:A:771:LEU:HD13	1:A:771:LEU:N	0.47	2.25	11	5
1:B:708:VAL:HG21	1:C:714:PRO:HD3	0.47	1.86	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:714:PRO:HB3	1:C:748:LEU:HD22	0.47	1.85	13	1
1:A:843:ILE:HD13	1:A:843:ILE:N	0.47	2.25	5	12
1:B:815:LEU:CB	1:B:830:ILE:HD11	0.47	2.40	14	2
1:A:771:LEU:HD22	1:A:771:LEU:N	0.47	2.24	15	8
1:C:764:SER:HB3	1:C:771:LEU:HD12	0.47	1.85	10	2
1:A:799:LEU:HD23	1:A:800:LEU:N	0.47	2.24	10	1
1:A:692:LEU:HD23	1:A:696:ARG:NE	0.47	2.23	13	1
1:C:710:GLN:O	1:C:710:GLN:HG3	0.47	2.10	13	1
1:C:713:SER:O	1:C:714:PRO:C	0.47	2.53	15	9
1:B:828:ARG:O	1:B:832:VAL:HG22	0.47	2.08	4	1
1:C:756:ILE:HD13	1:C:756:ILE:C	0.47	2.30	5	1
1:A:739:GLU:O	1:C:761:ARG:NE	0.47	2.48	13	1
1:B:806:GLU:CB	1:C:771:LEU:HD21	0.47	2.39	1	1
1:B:765:LEU:HD23	1:B:766:PHE:N	0.47	2.24	14	1
1:A:693:ILE:HD11	1:B:696:ARG:NE	0.47	2.24	8	1
1:C:756:ILE:O	1:C:760:LEU:HB2	0.47	2.09	8	1
1:C:850:GLY:O	1:C:854:ILE:HG22	0.46	2.09	4	3
1:A:696:ARG:O	1:A:699:PHE:HB2	0.46	2.11	11	2
1:C:704:LEU:HD22	1:C:707:ARG:CZ	0.46	2.41	6	1
1:C:792:ALA:HA	1:C:795:TYR:CE1	0.46	2.46	8	1
1:A:693:ILE:HD13	1:B:696:ARG:HG3	0.46	1.86	12	1
1:C:771:LEU:HD23	1:C:772:ARG:H	0.46	1.71	14	1
1:A:706:ASN:OD1	1:A:706:ASN:C	0.46	2.53	8	2
1:C:830:ILE:HD13	1:C:830:ILE:C	0.46	2.31	14	2
1:A:706:ASN:O	1:A:710:GLN:N	0.46	2.48	3	2
1:B:803:TRP:CH2	1:C:760:LEU:HD11	0.46	2.45	6	1
1:B:744:ARG:O	1:B:747:ARG:HB2	0.46	2.10	9	1
1:A:692:LEU:HD12	1:A:693:ILE:H	0.46	1.69	11	1
1:A:799:LEU:HD11	1:B:756:ILE:CG1	0.46	2.41	3	1
1:B:768:TYR:CE1	1:B:771:LEU:HD12	0.46	2.46	4	1
1:B:792:ALA:O	1:B:795:TYR:CD1	0.46	2.68	7	5
1:C:771:LEU:HD13	1:C:771:LEU:N	0.46	2.24	4	4
1:A:715:LEU:O	1:A:715:LEU:HD23	0.46	2.09	7	1
1:A:714:PRO:HA	1:C:704:LEU:HD12	0.46	1.88	10	1
1:C:774:LEU:CD1	1:C:777:ILE:HD11	0.46	2.40	13	1
1:A:756:ILE:HD12	1:C:799:LEU:HD13	0.46	1.86	1	1
1:A:790:TRP:C	1:A:792:ALA:N	0.46	2.67	7	6
1:C:777:ILE:HD13	1:C:777:ILE:C	0.46	2.31	2	1
1:B:790:TRP:C	1:B:792:ALA:N	0.46	2.68	11	14
1:B:795:TYR:CD1	1:C:753:LEU:HA	0.46	2.46	15	2
1:B:808:LYS:O	1:B:812:VAL:HG23	0.46	2.11	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:803:TRP:CZ2	1:C:763:LEU:HD22	0.46	2.45	4	1
1:A:746:ILE:O	1:A:749:VAL:HG23	0.46	2.10	10	1
1:A:758:ASP:HB3	1:B:715:LEU:HD21	0.46	1.87	3	1
1:B:799:LEU:HD13	1:B:800:LEU:HD22	0.46	1.85	3	1
1:B:830:ILE:HD13	1:B:830:ILE:C	0.46	2.31	3	3
1:A:706:ASN:OD1	1:A:707:ARG:N	0.46	2.48	7	4
1:A:819:ALA:HB1	1:A:826:THR:OG1	0.46	2.11	7	1
1:B:778:VAL:HG22	1:C:742:ARG:NH1	0.46	2.26	11	1
1:A:785:LEU:HD13	1:B:750:ASN:ND2	0.46	2.26	13	1
1:C:799:LEU:HG	1:C:803:TRP:CZ2	0.46	2.45	1	1
1:C:795:TYR:CE2	1:C:796:TRP:CD1	0.46	3.04	3	3
1:A:794:LYS:HE2	1:B:753:LEU:HD13	0.46	1.88	4	1
1:A:765:LEU:HD11	1:A:777:ILE:HD11	0.46	1.88	10	1
1:C:820:ILE:HD13	1:C:826:THR:OG1	0.46	2.10	6	1
1:C:791:GLU:O	1:C:795:TYR:CD1	0.46	2.69	7	2
1:B:793:LEU:HD22	1:B:797:TRP:CE2	0.46	2.46	12	1
1:B:799:LEU:HD13	1:B:800:LEU:H	0.46	1.70	12	1
1:A:774:LEU:HD13	1:A:774:LEU:C	0.46	2.30	13	1
1:B:713:SER:O	1:B:714:PRO:C	0.46	2.54	12	6
1:A:785:LEU:HD23	1:B:749:VAL:HB	0.46	1.87	2	2
1:C:768:TYR:C	1:C:770:ARG:H	0.46	2.14	2	1
1:A:775:LEU:HD23	1:A:776:LEU:H	0.46	1.71	3	2
1:B:774:LEU:HD11	1:C:742:ARG:NH2	0.46	2.26	9	1
1:A:756:ILE:HG22	1:C:799:LEU:HB2	0.45	1.87	5	1
1:A:812:VAL:HG21	1:A:834:GLN:HG3	0.45	1.87	10	1
1:A:816:ASN:N	1:A:830:ILE:HD11	0.45	2.26	10	1
1:B:692:LEU:O	1:B:695:LEU:CB	0.45	2.64	11	1
1:A:704:LEU:HD21	1:B:707:ARG:HB3	0.45	1.87	4	1
1:C:855:LEU:HD13	1:C:855:LEU:O	0.45	2.12	10	3
1:B:795:TYR:CZ	1:B:796:TRP:NE1	0.45	2.84	10	1
1:B:795:TYR:C	1:B:795:TYR:CD2	0.45	2.89	14	1
1:A:791:GLU:OE2	1:B:753:LEU:HD22	0.45	2.11	1	1
1:C:835:GLY:O	1:C:839:ALA:HB3	0.45	2.11	15	4
1:C:758:ASP:O	1:C:761:ARG:NE	0.45	2.50	8	1
1:A:715:LEU:O	1:A:716:SER:C	0.45	2.55	9	1
1:A:768:TYR:CE1	1:C:803:TRP:HA	0.45	2.47	13	1
1:B:690:GLY:O	1:B:693:ILE:HG23	0.45	2.11	11	2
1:A:760:LEU:HD23	1:A:760:LEU:C	0.45	2.32	12	3
1:A:799:LEU:HD11	1:B:756:ILE:HG12	0.45	1.87	3	1
1:A:755:LEU:HD13	1:B:715:LEU:HD21	0.45	1.87	4	1
1:B:705:VAL:HG21	1:B:748:LEU:CD2	0.45	2.41	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:774:LEU:HD21	1:C:742:ARG:NH2	0.45	2.26	9	1
1:A:785:LEU:HD13	1:B:750:ASN:OD1	0.45	2.11	13	1
1:A:781:ILE:HG12	1:B:746:ILE:HG21	0.45	1.88	7	1
1:B:843:ILE:HD12	1:B:843:ILE:N	0.45	2.26	15	1
1:C:753:LEU:C	1:C:753:LEU:HD12	0.45	2.31	1	2
1:A:802:TYR:CE2	1:B:768:TYR:CZ	0.45	3.05	2	1
1:A:698:VAL:O	1:A:701:VAL:HB	0.45	2.12	7	5
1:A:854:ILE:HG22	1:A:854:ILE:O	0.45	2.12	3	6
1:B:707:ARG:HD3	1:C:712:TYR:CZ	0.45	2.46	3	1
1:A:799:LEU:HD21	1:A:803:TRP:CH2	0.45	2.47	10	1
1:A:820:ILE:HD11	1:A:827:ASP:CB	0.45	2.42	14	1
1:B:799:LEU:HD21	1:C:760:LEU:CD1	0.45	2.42	2	1
1:A:745:SER:HA	1:A:748:LEU:HD22	0.45	1.86	5	1
1:A:744:ARG:O	1:A:748:LEU:HD23	0.45	2.12	9	1
1:A:774:LEU:CD2	1:A:777:ILE:HD11	0.45	2.42	14	1
1:B:707:ARG:NH1	1:C:712:TYR:CD1	0.45	2.85	15	1
1:C:750:ASN:ND2	1:C:750:ASN:H	0.45	2.10	15	1
1:A:785:LEU:HD21	1:B:750:ASN:ND2	0.45	2.27	7	2
1:B:832:VAL:O	1:B:836:ALA:HB2	0.45	2.12	3	6
1:A:770:ARG:O	1:A:774:LEU:N	0.45	2.49	9	2
1:C:704:LEU:HD22	1:C:707:ARG:NH1	0.45	2.27	10	1
1:A:812:VAL:HG13	1:A:816:ASN:ND2	0.45	2.27	13	1
1:B:768:TYR:CG	1:B:769:HIS:N	0.44	2.85	4	1
1:A:768:TYR:CE2	1:C:803:TRP:CE2	0.44	3.05	7	1
1:C:790:TRP:HA	1:C:790:TRP:CE3	0.44	2.47	7	2
1:A:785:LEU:HD22	1:B:749:VAL:HG13	0.44	1.87	13	1
1:A:705:VAL:HG22	1:A:748:LEU:HD23	0.44	1.88	1	1
1:A:814:LEU:O	1:A:818:THR:HG22	0.44	2.12	1	1
1:B:803:TRP:O	1:B:806:GLU:HG2	0.44	2.12	1	2
1:A:829:VAL:O	1:A:833:VAL:HG23	0.44	2.13	3	4
1:A:795:TYR:CD2	1:B:753:LEU:HA	0.44	2.47	7	1
1:A:756:ILE:O	1:A:760:LEU:HB2	0.44	2.11	7	2
1:B:812:VAL:HG12	1:B:816:ASN:ND2	0.44	2.27	3	1
1:C:795:TYR:CE1	1:C:796:TRP:CD1	0.44	3.05	5	3
1:B:712:TYR:CZ	1:C:712:TYR:OH	0.44	2.71	6	1
1:B:707:ARG:CZ	1:C:712:TYR:CE1	0.44	3.01	15	1
1:C:803:TRP:CE3	1:C:803:TRP:N	0.44	2.86	15	7
1:C:695:LEU:O	1:C:695:LEU:HD23	0.44	2.12	6	1
1:C:697:ILE:HD13	1:C:697:ILE:C	0.44	2.33	7	1
1:C:758:ASP:O	1:C:761:ARG:CZ	0.44	2.65	7	2
1:A:695:LEU:C	1:A:695:LEU:HD23	0.44	2.33	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:692:LEU:O	1:B:696:ARG:NH1	0.44	2.51	11	1
1:A:768:TYR:CE2	1:C:803:TRP:CE3	0.44	3.06	13	1
1:A:835:GLY:O	1:A:839:ALA:HB3	0.44	2.12	6	2
1:A:854:ILE:O	1:A:854:ILE:HD13	0.44	2.13	1	1
1:C:771:LEU:H	1:C:771:LEU:HD22	0.44	1.72	6	2
1:B:847:ILE:HG23	1:B:848:ARG:N	0.44	2.28	15	4
1:B:808:LYS:O	1:B:812:VAL:HG12	0.44	2.13	10	1
1:C:774:LEU:HD13	1:C:777:ILE:CD1	0.44	2.43	13	1
1:C:795:TYR:CZ	1:C:796:TRP:CE2	0.44	3.05	14	1
1:B:828:ARG:O	1:B:832:VAL:HG23	0.44	2.12	15	1
1:B:771:LEU:N	1:B:771:LEU:HD22	0.44	2.28	1	4
1:A:715:LEU:O	1:C:754:ALA:HB1	0.44	2.13	2	1
1:B:790:TRP:CE3	1:B:790:TRP:HA	0.44	2.48	15	7
1:B:705:VAL:HG21	1:B:748:LEU:HD12	0.44	1.88	6	1
1:B:795:TYR:CD2	1:C:756:ILE:HB	0.44	2.47	1	1
1:B:793:LEU:O	1:B:797:TRP:CD1	0.44	2.71	8	4
1:C:744:ARG:CZ	1:C:747:ARG:HB2	0.44	2.42	5	1
1:A:763:LEU:H	1:A:763:LEU:HD13	0.44	1.73	9	1
1:A:756:ILE:HD13	1:C:795:TYR:O	0.44	2.13	10	1
1:C:777:ILE:HD12	1:C:781:ILE:HD13	0.44	1.90	15	1
1:B:695:LEU:O	1:B:698:VAL:HG12	0.44	2.13	7	2
1:A:768:TYR:CD1	1:C:803:TRP:HA	0.44	2.48	10	1
1:C:690:GLY:O	1:C:693:ILE:HG23	0.44	2.13	11	2
1:C:758:ASP:O	1:C:761:ARG:HD2	0.44	2.13	11	1
1:B:794:LYS:NZ	1:C:753:LEU:HD13	0.44	2.28	15	1
1:C:794:LYS:HD3	1:C:795:TYR:N	0.43	2.28	1	2
1:B:836:ALA:O	1:B:840:ILE:HG22	0.43	2.13	3	2
1:B:822:VAL:O	1:B:822:VAL:HG13	0.43	2.13	4	1
1:B:828:ARG:O	1:B:832:VAL:HG12	0.43	2.13	5	5
1:B:799:LEU:O	1:B:803:TRP:CD2	0.43	2.71	7	1
1:B:747:ARG:O	1:B:751:GLY:N	0.43	2.51	9	1
1:A:756:ILE:HD13	1:C:795:TYR:OH	0.43	2.12	13	1
1:B:820:ILE:HD12	1:B:820:ILE:N	0.43	2.28	14	2
1:A:768:TYR:CZ	1:A:771:LEU:HD11	0.43	2.48	9	1
1:C:764:SER:C	1:C:774:LEU:HD11	0.43	2.33	11	1
1:B:763:LEU:O	1:B:774:LEU:HD22	0.43	2.13	15	1
1:B:741:ASP:O	1:B:744:ARG:N	0.43	2.50	12	4
1:B:819:ALA:HB1	1:B:827:ASP:N	0.43	2.27	11	1
1:B:795:TYR:CE2	1:C:756:ILE:HD13	0.43	2.48	12	1
1:B:799:LEU:CB	1:C:760:LEU:HD11	0.43	2.42	12	1
1:A:749:VAL:CG2	1:C:785:LEU:HD11	0.43	2.44	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:758:ASP:N	1:A:758:ASP:OD1	0.43	2.51	6	1
1:C:774:LEU:O	1:C:778:VAL:HG23	0.43	2.13	6	1
1:B:704:LEU:HD21	1:C:707:ARG:HA	0.43	1.90	7	1
1:A:693:ILE:HD13	1:B:696:ARG:HH11	0.43	1.69	11	1
1:B:692:LEU:O	1:B:696:ARG:NH2	0.43	2.51	5	1
1:A:790:TRP:CE3	1:A:790:TRP:HA	0.43	2.49	7	1
1:B:799:LEU:HD23	1:C:756:ILE:HG12	0.43	1.91	7	1
1:A:800:LEU:HD13	1:A:800:LEU:O	0.43	2.13	8	1
1:A:768:TYR:CE1	1:A:771:LEU:CD2	0.43	3.01	10	1
1:A:748:LEU:HD12	1:A:748:LEU:O	0.43	2.13	13	1
1:A:713:SER:OG	1:C:708:VAL:HG22	0.43	2.12	14	1
1:B:693:ILE:HD12	1:C:696:ARG:HE	0.43	1.72	15	1
1:A:705:VAL:HG22	1:A:748:LEU:CD2	0.43	2.44	1	1
1:B:795:TYR:CE2	1:B:796:TRP:NE1	0.43	2.86	1	1
1:B:781:ILE:HG12	1:B:785:LEU:HD13	0.43	1.90	2	1
1:A:799:LEU:HD13	1:B:756:ILE:HG21	0.43	1.91	5	1
1:A:747:ARG:CZ	1:C:785:LEU:HB3	0.43	2.43	10	1
1:A:693:ILE:HD13	1:B:696:ARG:CD	0.43	2.43	15	1
1:A:712:TYR:HH	1:C:712:TYR:HD2	0.43	1.54	2	1
1:A:771:LEU:HD23	1:A:772:ARG:HD3	0.43	1.89	2	1
1:B:792:ALA:HA	1:B:795:TYR:CE1	0.43	2.48	3	1
1:A:753:LEU:C	1:A:753:LEU:HD12	0.43	2.34	13	1
1:C:774:LEU:HD13	1:C:777:ILE:HD11	0.43	1.90	13	1
1:A:756:ILE:HD11	1:C:795:TYR:HB2	0.43	1.90	1	1
1:C:815:LEU:HD23	1:C:830:ILE:HD11	0.43	1.89	1	1
1:A:693:ILE:HD13	1:B:693:ILE:CG1	0.43	2.44	2	1
1:B:710:GLN:O	1:B:715:LEU:HD11	0.43	2.14	2	1
1:B:781:ILE:CG1	1:B:785:LEU:HD13	0.43	2.44	2	1
1:C:833:VAL:HG23	1:C:834:GLN:N	0.43	2.29	10	5
1:A:692:LEU:HD23	1:A:696:ARG:HH11	0.43	1.74	10	1
1:A:693:ILE:HB	1:B:696:ARG:CZ	0.43	2.44	11	1
1:A:768:TYR:O	1:A:771:LEU:HG	0.43	2.14	1	1
1:A:795:TYR:CB	1:B:756:ILE:HG21	0.43	2.44	3	1
1:B:799:LEU:HB2	1:C:756:ILE:HD11	0.43	1.89	3	1
1:A:807:LEU:HD22	1:B:772:ARG:NH1	0.43	2.28	6	1
1:A:771:LEU:CD1	1:A:771:LEU:H	0.43	2.26	8	1
1:B:796:TRP:HA	1:B:799:LEU:HD12	0.43	1.91	12	1
1:A:746:ILE:CG2	1:C:781:ILE:HG23	0.42	2.41	1	1
1:A:802:TYR:CZ	1:B:760:LEU:HD11	0.42	2.49	1	2
1:C:771:LEU:N	1:C:771:LEU:HD13	0.42	2.29	7	2
1:C:820:ILE:N	1:C:820:ILE:HD12	0.42	2.28	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:693:ILE:C	1:A:693:ILE:HD12	0.42	2.34	10	1
1:B:753:LEU:C	1:B:753:LEU:HD12	0.42	2.33	14	1
1:A:756:ILE:HD13	1:C:796:TRP:CD1	0.42	2.49	1	1
1:C:829:VAL:O	1:C:833:VAL:HG12	0.42	2.14	1	1
1:B:763:LEU:O	1:B:774:LEU:HD12	0.42	2.14	9	1
1:B:771:LEU:O	1:B:774:LEU:HG	0.42	2.14	10	1
1:A:757:TRP:CD1	1:A:758:ASP:N	0.42	2.87	14	1
1:B:815:LEU:HB2	1:B:830:ILE:HD11	0.42	1.91	14	1
1:B:781:ILE:HD12	1:B:782:VAL:H	0.42	1.70	15	1
1:C:795:TYR:HD2	1:C:796:TRP:N	0.42	2.12	1	1
1:A:802:TYR:CE1	1:B:760:LEU:HD11	0.42	2.50	2	1
1:A:771:LEU:HD13	1:A:771:LEU:H	0.42	1.73	6	1
1:A:808:LYS:HZ3	1:A:838:ARG:N	0.42	2.11	6	1
1:B:763:LEU:HD23	1:B:764:SER:N	0.42	2.27	10	3
1:A:748:LEU:O	1:B:716:SER:CB	0.42	2.68	9	1
1:A:793:LEU:HD13	1:A:793:LEU:O	0.42	2.14	2	1
1:A:742:ARG:O	1:A:746:ILE:HD12	0.42	2.15	6	1
1:A:750:ASN:N	1:C:785:LEU:HD21	0.42	2.29	6	1
1:A:795:TYR:CD2	1:B:756:ILE:CG2	0.42	3.00	8	1
1:A:709:ARG:CZ	1:A:709:ARG:HA	0.42	2.45	9	1
1:C:771:LEU:HD23	1:C:772:ARG:CD	0.42	2.45	2	1
1:B:781:ILE:HD13	1:C:746:ILE:CG2	0.42	2.43	15	1
1:C:822:VAL:HG13	1:C:823:GLY:N	0.42	2.30	11	5
1:C:816:ASN:O	1:C:820:ILE:HD13	0.42	2.15	5	1
1:B:769:HIS:H	1:B:771:LEU:HD12	0.42	1.75	12	1
1:A:765:LEU:HD12	1:A:765:LEU:N	0.42	2.30	1	1
1:A:815:LEU:O	1:A:819:ALA:HB2	0.42	2.15	1	1
1:B:760:LEU:HD23	1:B:760:LEU:O	0.42	2.14	1	2
1:A:800:LEU:HA	1:A:803:TRP:CE3	0.42	2.49	6	2
1:A:758:ASP:CB	1:B:715:LEU:HD21	0.42	2.45	3	1
1:A:710:GLN:O	1:A:715:LEU:HD12	0.42	2.15	5	1
1:B:695:LEU:HD23	1:B:695:LEU:C	0.42	2.35	3	3
1:A:771:LEU:CD1	1:A:772:ARG:N	0.42	2.82	7	1
1:B:830:ILE:HG23	1:B:831:GLU:N	0.42	2.30	8	2
1:A:815:LEU:CB	1:A:830:ILE:HD13	0.42	2.45	12	1
1:B:763:LEU:C	1:B:763:LEU:HD23	0.42	2.35	9	2
1:B:771:LEU:HD13	1:B:771:LEU:N	0.42	2.27	1	1
1:A:780:ARG:O	1:A:784:LEU:HD23	0.42	2.15	2	1
1:B:791:GLU:O	1:B:795:TYR:CD1	0.42	2.73	3	1
1:A:820:ILE:O	1:A:821:ALA:O	0.42	2.37	5	1
1:C:793:LEU:O	1:C:797:TRP:CD1	0.42	2.73	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:793:LEU:HD23	1:B:847:ILE:HG12	0.42	1.91	10	1
1:A:774:LEU:O	1:A:777:ILE:HG13	0.42	2.15	11	2
1:C:777:ILE:HD12	1:C:777:ILE:C	0.42	2.35	13	1
1:A:714:PRO:HD2	1:C:708:VAL:HG21	0.41	1.92	3	1
1:C:744:ARG:O	1:C:747:ARG:HB2	0.41	2.15	14	2
1:A:753:LEU:HD13	1:C:791:GLU:HB3	0.41	1.91	13	1
1:C:799:LEU:O	1:C:803:TRP:CG	0.41	2.73	13	1
1:C:771:LEU:N	1:C:771:LEU:HD22	0.41	2.29	15	1
1:A:746:ILE:HG22	1:C:785:LEU:HD22	0.41	1.92	1	1
1:C:847:ILE:N	1:C:847:ILE:HD13	0.41	2.29	12	3
1:A:771:LEU:H	1:A:771:LEU:CD1	0.41	2.28	5	1
1:A:756:ILE:N	1:A:756:ILE:HD12	0.41	2.30	13	1
1:A:765:LEU:HD23	1:A:766:PHE:N	0.41	2.29	2	1
1:A:847:ILE:C	1:A:847:ILE:HD12	0.41	2.35	2	1
1:A:830:ILE:HD12	1:A:831:GLU:N	0.41	2.30	3	1
1:A:715:LEU:HD22	1:C:754:ALA:HB1	0.41	1.92	13	1
1:A:799:LEU:HD23	1:A:803:TRP:HZ2	0.41	1.72	15	1
1:C:742:ARG:O	1:C:746:ILE:HD13	0.41	2.15	15	1
1:C:764:SER:C	1:C:774:LEU:HD12	0.41	2.36	6	1
1:A:795:TYR:CE2	1:B:757:TRP:CD1	0.41	3.09	12	1
1:C:750:ASN:N	1:C:750:ASN:ND2	0.41	2.68	14	1
1:B:803:TRP:O	1:B:806:GLU:HG3	0.41	2.15	15	1
1:B:744:ARG:O	1:B:747:ARG:HB3	0.41	2.16	5	1
1:C:774:LEU:O	1:C:777:ILE:CG1	0.41	2.69	8	1
1:A:743:ASP:HA	1:A:746:ILE:HD12	0.41	1.91	9	1
1:A:775:LEU:HD23	1:A:775:LEU:C	0.41	2.36	9	1
1:C:703:SER:O	1:C:707:ARG:HD2	0.41	2.16	9	1
1:C:790:TRP:C	1:C:792:ALA:H	0.41	2.18	9	1
1:C:707:ARG:HA	1:C:712:TYR:CD2	0.41	2.50	15	1
1:A:793:LEU:HD21	1:A:847:ILE:HD11	0.41	1.91	4	1
1:C:746:ILE:HD12	1:C:746:ILE:N	0.41	2.31	9	1
1:A:696:ARG:HD2	1:A:696:ARG:N	0.41	2.31	2	1
1:C:708:VAL:HG12	1:C:741:ASP:OD2	0.41	2.16	5	1
1:B:836:ALA:O	1:B:840:ILE:HD12	0.41	2.15	12	2
1:A:696:ARG:N	1:A:696:ARG:HD3	0.41	2.29	8	1
1:A:692:LEU:HD23	1:A:696:ARG:NH1	0.41	2.31	10	1
1:B:764:SER:CB	1:B:771:LEU:HD12	0.41	2.46	13	2
1:A:768:TYR:OH	1:A:771:LEU:CD2	0.41	2.69	13	1
1:B:791:GLU:CB	1:C:753:LEU:HD22	0.41	2.43	1	1
1:B:706:ASN:O	1:B:710:GLN:N	0.41	2.54	2	1
1:A:760:LEU:HA	1:A:763:LEU:HD11	0.41	1.91	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:833:VAL:HG13	1:B:834:GLN:N	0.41	2.31	7	1
1:A:768:TYR:CZ	1:C:803:TRP:CD2	0.41	3.08	13	1
1:B:763:LEU:HA	1:B:774:LEU:HD22	0.41	1.92	15	1
1:C:790:TRP:O	1:C:792:ALA:N	0.41	2.53	7	3
1:B:756:ILE:HD11	1:B:760:LEU:HD13	0.41	1.92	3	1
1:B:818:THR:O	1:B:821:ALA:HB3	0.41	2.15	4	1
1:B:744:ARG:NH2	1:C:716:SER:OG	0.41	2.53	6	1
1:B:795:TYR:CD2	1:B:796:TRP:CD1	0.41	3.09	6	1
1:B:803:TRP:HH2	1:C:760:LEU:HD11	0.41	1.75	6	1
1:A:704:LEU:HD13	1:B:707:ARG:HG3	0.41	1.93	9	1
1:C:856:LEU:C	1:C:856:LEU:HD12	0.41	2.36	10	2
1:B:830:ILE:CG2	1:B:831:GLU:N	0.41	2.83	11	1
1:A:766:PHE:O	1:A:767:SER:CB	0.41	2.69	13	1
1:A:776:LEU:O	1:A:779:THR:HG22	0.41	2.16	14	1
1:C:830:ILE:HG23	1:C:831:GLU:N	0.41	2.30	5	3
1:A:756:ILE:HB	1:C:795:TYR:HB2	0.41	1.92	6	1
1:C:781:ILE:HD13	1:C:785:LEU:HD13	0.41	1.90	8	1
1:C:764:SER:O	1:C:765:LEU:CB	0.41	2.69	9	1
1:A:693:ILE:HD13	1:B:693:ILE:HG12	0.41	1.93	10	1
1:B:755:LEU:HD23	1:B:755:LEU:O	0.41	2.16	14	1
1:A:802:TYR:CZ	1:B:768:TYR:OH	0.40	2.74	1	1
1:A:765:LEU:O	1:A:766:PHE:O	0.40	2.39	10	1
1:C:847:ILE:HD13	1:C:847:ILE:H	0.40	1.76	2	1
1:A:753:LEU:O	1:A:756:ILE:HG22	0.40	2.17	3	1
1:A:806:GLU:CB	1:B:768:TYR:OH	0.40	2.70	4	1
1:B:813:SER:O	1:B:817:ALA:HB2	0.40	2.16	4	1
1:A:776:LEU:O	1:A:776:LEU:HD23	0.40	2.17	5	1
1:C:843:ILE:HD12	1:C:844:PRO:O	0.40	2.16	6	1
1:A:704:LEU:HD13	1:B:707:ARG:CG	0.40	2.46	9	1
1:A:795:TYR:CD2	1:A:795:TYR:C	0.40	2.95	10	1
1:B:704:LEU:HD22	1:B:704:LEU:N	0.40	2.32	10	1
1:C:820:ILE:HD12	1:C:827:ASP:HB2	0.40	1.93	10	1
1:A:774:LEU:HD23	1:A:774:LEU:C	0.40	2.37	11	1
1:C:855:LEU:O	1:C:855:LEU:HD13	0.40	2.16	11	1
1:C:795:TYR:CD1	1:C:796:TRP:CD1	0.40	3.09	12	1
1:A:781:ILE:HD12	1:B:746:ILE:CD1	0.40	2.46	13	1
1:C:856:LEU:HD12	1:C:856:LEU:C	0.40	2.36	13	1
1:A:795:TYR:CD1	1:A:796:TRP:CD1	0.40	3.09	1	1
1:C:833:VAL:HG13	1:C:834:GLN:N	0.40	2.31	1	1
1:C:832:VAL:O	1:C:836:ALA:HB2	0.40	2.16	2	1
1:B:814:LEU:HD23	1:B:814:LEU:C	0.40	2.37	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:816:ASN:CB	1:A:830:ILE:HD11	0.40	2.46	8	1
1:A:781:ILE:O	1:A:785:LEU:HD13	0.40	2.16	10	1
1:A:762:SER:O	1:A:774:LEU:HD13	0.40	2.16	14	1
1:B:830:ILE:HD13	1:B:834:GLN:NE2	0.40	2.32	14	1
1:A:710:GLN:HG2	1:C:704:LEU:HD21	0.40	1.93	15	1
1:A:760:LEU:C	1:A:760:LEU:HD23	0.40	2.36	15	1
1:B:799:LEU:HD22	1:B:803:TRP:CH2	0.40	2.52	2	1
1:B:832:VAL:HG23	1:B:833:VAL:N	0.40	2.31	2	1
1:B:703:SER:O	1:B:707:ARG:HD2	0.40	2.16	3	1
1:C:795:TYR:CE2	1:C:796:TRP:NE1	0.40	2.90	4	1
1:A:821:ALA:O	1:A:822:VAL:CG2	0.40	2.69	5	1
1:C:807:LEU:O	1:C:807:LEU:HD13	0.40	2.16	9	1
1:A:751:GLY:O	1:A:755:LEU:N	0.40	2.53	10	1
1:A:697:ILE:HD11	1:B:696:ARG:CD	0.40	2.46	13	1
1:A:742:ARG:NH1	1:C:778:VAL:HG12	0.40	2.31	13	1
1:A:820:ILE:HD11	1:A:827:ASP:HB3	0.40	1.91	14	1
1:A:795:TYR:CD1	1:B:753:LEU:O	0.40	2.74	15	1
1:A:756:ILE:HG23	1:A:757:TRP:N	0.40	2.32	3	1
1:C:847:ILE:HD13	1:C:847:ILE:N	0.40	2.32	7	1
1:A:702:LEU:O	1:A:705:VAL:CG2	0.40	2.69	11	1
1:B:856:LEU:O	1:B:856:LEU:HD23	0.40	2.17	13	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	140/180 (78%)	128±2 (91±1%)	7±2 (5±1%)	6±2 (4±1%)	5	30
1	B	143/180 (79%)	129±2 (90±1%)	7±1 (5±1%)	7±2 (5±1%)	4	26
1	C	142/180 (79%)	129±2 (91±2%)	6±2 (4±1%)	7±1 (5±1%)	4	26
All	All	6375/8100 (79%)	5787 (91%)	291 (5%)	297 (5%)	4	27

All 53 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.



Mol	Chain	Res	Type	Models (Total)
1	B	741	ASP	15
1	C	821	ALA	15
1	B	714	PRO	14
1	B	844	PRO	14
1	C	714	PRO	12
1	A	714	PRO	11
1	A	821	ALA	11
1	A	822	VAL	10
1	B	712	TYR	10
1	C	765	LEU	10
1	C	825	GLY	10
1	C	822	VAL	10
1	C	769	HIS	9
1	A	712	TYR	8
1	A	768	TYR	8
1	C	711	GLY	8
1	A	741	ASP	7
1	B	768	TYR	7
1	B	843	ILE	7
1	A	767	SER	6
1	B	825	GLY	6
1	B	767	SER	6
1	C	741	ASP	6
1	B	765	LEU	6
1	C	846	ARG	6
1	B	824	GLU	5
1	A	715	LEU	4
1	C	712	TYR	4
1	C	844	PRO	4
1	A	825	GLY	4
1	A	765	LEU	4
1	A	824	GLU	3
1	B	769	HIS	3
1	B	766	PHE	3
1	B	823	GLY	3
1	C	768	TYR	2
1	C	845	ARG	2
1	C	824	GLU	2
1	B	845	ARG	2
1	A	823	GLY	2
1	A	711	GLY	2
1	A	844	PRO	2
1	B	822	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	766	PHE	2
1	A	845	ARG	2
1	B	846	ARG	1
1	C	767	SER	1
1	C	823	GLY	1
1	A	769	HIS	1
1	A	846	ARG	1
1	C	842	HIS	1
1	B	842	HIS	1
1	C	766	PHE	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	125/157 (80%)	92±3 (73±2%)	33±3 (27±2%)	2	22
1	B	127/157 (81%)	99±4 (78±3%)	28±4 (22±3%)	3	30
1	C	126/157 (80%)	98±3 (78±2%)	28±3 (22±2%)	3	29
All	All	5670/7065 (80%)	4325 (76%)	1345 (24%)	2	27

All 288 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	794	LYS	15
1	A	843	ILE	15
1	B	693	ILE	15
1	B	771	LEU	15
1	B	794	LYS	15
1	C	771	LEU	15
1	C	794	LYS	15
1	C	803	TRP	15
1	A	744	ARG	14
1	A	763	LEU	14
1	A	771	LEU	14
1	B	803	TRP	14
1	B	838	ARG	14

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Mol	Chain	Res	Type	Models (Total)
1	A	692	LEU	13
1	A	775	LEU	13
1	A	799	LEU	13
1	A	855	LEU	13
1	B	830	ILE	12
1	C	838	ARG	12
1	C	855	LEU	12
1	A	797	TRP	12
1	C	761	ARG	12
1	A	772	ARG	12
1	A	800	LEU	11
1	B	834	GLN	11
1	C	772	ARG	11
1	A	697	ILE	10
1	A	761	ARG	10
1	B	757	TRP	10
1	C	764	SER	10
1	C	847	ILE	10
1	A	757	TRP	10
1	A	784	LEU	10
1	A	795	TYR	10
1	A	747	ARG	9
1	B	747	ARG	9
1	B	784	LEU	9
1	B	848	ARG	9
1	C	788	ARG	9
1	A	773	ASP	9
1	A	806	GLU	9
1	B	715	LEU	9
1	B	774	LEU	9
1	B	790	TRP	9
1	C	693	ILE	9
1	C	697	ILE	9
1	B	692	LEU	9
1	B	713	SER	9
1	A	768	TYR	8
1	A	803	TRP	8
1	B	756	ILE	8
1	B	768	TYR	8
1	B	799	LEU	8
1	C	716	SER	8
1	C	744	ARG	8

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Mol	Chain	Res	Type	Models (Total)
1	C	770	ARG	8
1	C	795	TYR	8
1	A	764	SER	8
1	A	856	LEU	8
1	C	826	THR	8
1	A	765	LEU	8
1	C	790	TRP	8
1	C	807	LEU	8
1	C	704	LEU	8
1	C	753	LEU	8
1	A	712	TYR	7
1	A	802	TYR	7
1	B	691	SER	7
1	B	742	ARG	7
1	B	772	ARG	7
1	C	692	LEU	7
1	C	758	ASP	7
1	C	834	GLN	7
1	B	712	TYR	7
1	B	842	HIS	7
1	B	709	ARG	7
1	A	709	ARG	6
1	A	742	ARG	6
1	A	758	ASP	6
1	A	814	LEU	6
1	A	841	ARG	6
1	B	780	ARG	6
1	C	774	LEU	6
1	A	752	SER	6
1	A	780	ARG	6
1	A	805	GLN	6
1	A	830	ILE	6
1	B	765	LEU	6
1	C	777	ILE	6
1	C	740	ARG	6
1	C	773	ASP	6
1	A	756	ILE	6
1	A	838	ARG	6
1	A	822	VAL	5
1	B	755	LEU	5
1	B	791	GLU	5
1	C	748	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	C	752	SER	5
1	C	755	LEU	5
1	B	739	GLU	5
1	B	745	SER	5
1	B	746	ILE	5
1	B	764	SER	5
1	A	793	LEU	5
1	B	761	ARG	5
1	B	770	ARG	5
1	B	773	ASP	5
1	C	709	ARG	5
1	C	712	TYR	5
1	C	715	LEU	5
1	A	707	ARG	5
1	A	706	ASN	5
1	C	801	GLN	5
1	A	767	SER	4
1	B	740	ARG	4
1	B	741	ASP	4
1	B	805	GLN	4
1	C	780	ARG	4
1	A	695	LEU	4
1	A	708	VAL	4
1	A	740	ARG	4
1	B	697	ILE	4
1	C	710	GLN	4
1	C	775	LEU	4
1	A	715	LEU	4
1	A	776	LEU	4
1	C	707	ARG	4
1	C	848	ARG	4
1	B	814	LEU	4
1	B	846	ARG	4
1	A	774	LEU	4
1	B	753	LEU	4
1	C	741	ASP	4
1	C	842	HIS	4
1	A	713	SER	3
1	A	716	SER	3
1	A	741	ASP	3
1	B	704	LEU	3
1	B	795	TYR	3

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Mol	Chain	Res	Type	Models (Total)
1	B	808	LYS	3
1	B	809	ASN	3
1	B	851	LEU	3
1	C	696	ARG	3
1	C	760	LEU	3
1	C	765	LEU	3
1	C	853	ARG	3
1	A	750	ASN	3
1	A	812	VAL	3
1	B	707	ARG	3
1	B	806	GLU	3
1	C	702	LEU	3
1	C	742	ARG	3
1	C	756	ILE	3
1	C	757	TRP	3
1	C	799	LEU	3
1	C	830	ILE	3
1	A	748	LEU	3
1	A	807	LEU	3
1	A	824	GLU	3
1	A	834	GLN	3
1	B	743	ASP	3
1	B	841	ARG	3
1	C	781	ILE	3
1	A	704	LEU	3
1	A	809	ASN	3
1	A	826	THR	3
1	B	703	SER	3
1	B	760	LEU	3
1	B	816	ASN	3
1	B	845	ARG	3
1	C	745	SER	3
1	B	716	SER	3
1	B	744	ARG	3
1	B	826	THR	3
1	C	713	SER	3
1	C	806	GLU	3
1	C	849	GLN	3
1	A	693	ILE	3
1	C	800	LEU	3
1	C	703	SER	3
1	B	696	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	C	766	PHE	3
1	A	703	SER	2
1	A	743	ASP	2
1	B	710	GLN	2
1	C	699	PHE	2
1	C	708	VAL	2
1	C	810	SER	2
1	C	851	LEU	2
1	A	770	ARG	2
1	B	762	SER	2
1	B	767	SER	2
1	B	793	LEU	2
1	A	755	LEU	2
1	A	816	ASN	2
1	C	747	ARG	2
1	C	816	ASN	2
1	B	849	GLN	2
1	C	691	SER	2
1	A	791	GLU	2
1	A	820	ILE	2
1	B	847	ILE	2
1	A	698	VAL	2
1	A	798	ASN	2
1	A	849	GLN	2
1	C	805	GLN	2
1	A	760	LEU	2
1	A	790	TRP	2
1	A	739	GLU	2
1	B	785	LEU	2
1	B	856	LEU	2
1	C	852	GLU	2
1	A	762	SER	2
1	A	781	ILE	2
1	A	783	GLU	2
1	B	702	LEU	2
1	C	759	ASP	2
1	B	763	LEU	2
1	B	766	PHE	2
1	A	701	VAL	2
1	A	714	PRO	2
1	B	748	LEU	2
1	C	837	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	C	827	ASP	2
1	C	750	ASN	2
1	A	854	ILE	1
1	B	714	PRO	1
1	B	758	ASP	1
1	C	793	LEU	1
1	C	802	TYR	1
1	C	815	LEU	1
1	C	831	GLU	1
1	A	696	ARG	1
1	A	804	SER	1
1	A	810	SER	1
1	B	769	HIS	1
1	B	798	ASN	1
1	B	801	GLN	1
1	C	762	SER	1
1	C	769	HIS	1
1	C	783	GLU	1
1	C	791	GLU	1
1	C	840	ILE	1
1	A	766	PHE	1
1	A	777	ILE	1
1	B	800	LEU	1
1	B	804	SER	1
1	B	853	ARG	1
1	A	845	ARG	1
1	B	831	GLU	1
1	B	837	SER	1
1	C	856	LEU	1
1	A	846	ARG	1
1	C	695	LEU	1
1	C	804	SER	1
1	C	812	VAL	1
1	A	746	ILE	1
1	B	699	PHE	1
1	B	782	VAL	1
1	C	813	SER	1
1	C	798	ASN	1
1	B	779	THR	1
1	B	797	TRP	1
1	C	698	VAL	1
1	C	787	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	699	PHE	1
1	A	705	VAL	1
1	A	785	LEU	1
1	A	745	SER	1
1	A	837	SER	1
1	B	852	GLU	1
1	C	808	LYS	1
1	A	753	LEU	1
1	A	848	ARG	1
1	A	851	LEU	1
1	C	739	GLU	1
1	C	763	LEU	1
1	C	767	SER	1
1	C	845	ARG	1
1	A	702	LEU	1
1	A	749	VAL	1
1	A	852	GLU	1
1	B	706	ASN	1
1	B	822	VAL	1
1	A	827	ASP	1
1	A	831	GLU	1
1	B	855	LEU	1
1	C	779	THR	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

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\_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	596
Number of shifts mapped to atoms	596
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
$^{13}\text{C}_\alpha$	157	$-0.02 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	145	$-0.29 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	147	$0.80 \pm 0.18$	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. 508 atoms were assigned a chemical shift out of a possible 5791. 0 out of 115 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	508/2158 (24%)	126/862 (15%)	256/868 (29%)	126/428 (29%)
Sidechain	0/3255 (0%)	0/1894 (0%)	0/1145 (0%)	0/216 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/378 (0%)	0/192 (0%)	0/159 (0%)	0/27 (0%)
Overall	508/5791 (9%)	126/2948 (4%)	256/2172 (12%)	126/671 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 561 atoms were assigned a chemical shift out of a possible 6402. 0 out of 120 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	561/2358 (24%)	139/942 (15%)	283/948 (30%)	139/468 (30%)
Sidechain	0/3543 (0%)	0/2061 (0%)	0/1254 (0%)	0/228 (0%)
Aromatic	0/501 (0%)	0/255 (0%)	0/213 (0%)	0/33 (0%)
Overall	561/6402 (9%)	139/3258 (4%)	283/2415 (12%)	139/729 (19%)

#### 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:

