



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2022 – 03:46 AM EST

PDB ID : 6UJV
Title : Model of the HIV-1 gp41 membrane-proximal external region, transmembrane domain and cytoplasmic tail (LLP2)
Authors : Piai, A.; Fu, Q.; Cai, Y.; Ghantous, F.; Xiao, T.; Shaik, M.M.; Peng, H.; Rits-Volloch, S.; Liu, Z.; Chen, W.; Seaman, M.S.; Chen, B.; Chou, J.J.
Deposited on : 2019-10-03

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

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	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

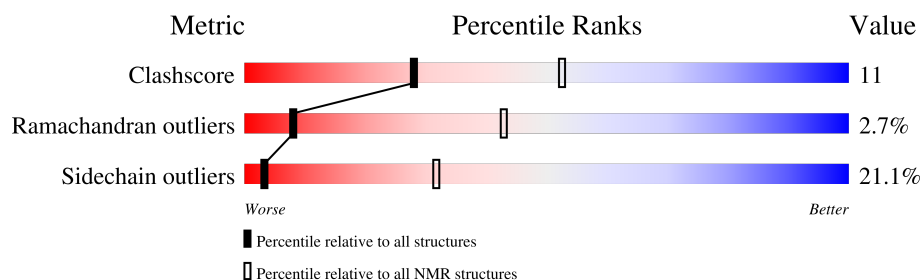
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 10%.

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 ≥ 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	129	
1	B	129	
1	C	129	

2 Ensemble composition and analysis

This entry contains 15 models. Model 9 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:785, B:660-B:716, B:739-B:788, C:660-C:716, C:739-C:783 (313)	0.60	9

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

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

The models can be grouped into 2 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5577 atoms, of which 2859 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein GP41.

Mol	Chain	Residues	Atoms					Trace
1	A	107	Total	C	H	N	O	0
			1859	595	953	163	148	
1	B	107	Total	C	H	N	O	0
			1859	595	953	163	148	
1	C	107	Total	C	H	N	O	0
			1859	595	953	163	148	

There are 21 discrepancies between the modelled and reference sequences:

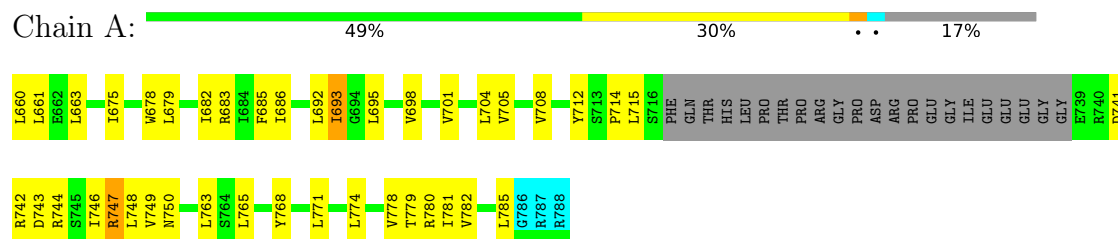
Chain	Residue	Modelled	Actual	Comment	Reference
A	683	ARG	LYS	conflict	UNP A0A060KRW4
A	684	ILE	LEU	conflict	UNP A0A060KRW4
A	687	ILE	MET	conflict	UNP A0A060KRW4
A	691	SER	GLY	conflict	UNP A0A060KRW4
A	704	LEU	ILE	conflict	UNP A0A060KRW4
A	723	THR	ILE	conflict	UNP A0A060KRW4
A	764	SER	CYS	engineered mutation	UNP A0A060KRW4
B	683	ARG	LYS	conflict	UNP A0A060KRW4
B	684	ILE	LEU	conflict	UNP A0A060KRW4
B	687	ILE	MET	conflict	UNP A0A060KRW4
B	691	SER	GLY	conflict	UNP A0A060KRW4
B	704	LEU	ILE	conflict	UNP A0A060KRW4
B	723	THR	ILE	conflict	UNP A0A060KRW4
B	764	SER	CYS	engineered mutation	UNP A0A060KRW4
C	683	ARG	LYS	conflict	UNP A0A060KRW4
C	684	ILE	LEU	conflict	UNP A0A060KRW4
C	687	ILE	MET	conflict	UNP A0A060KRW4
C	691	SER	GLY	conflict	UNP A0A060KRW4
C	704	LEU	ILE	conflict	UNP A0A060KRW4
C	723	THR	ILE	conflict	UNP A0A060KRW4
C	764	SER	CYS	engineered mutation	UNP A0A060KRW4

4 Residue-property plots

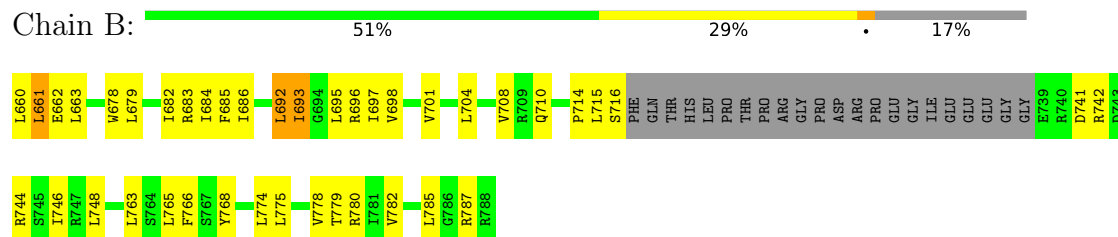
4.1 Average score per residue in the NMR ensemble

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

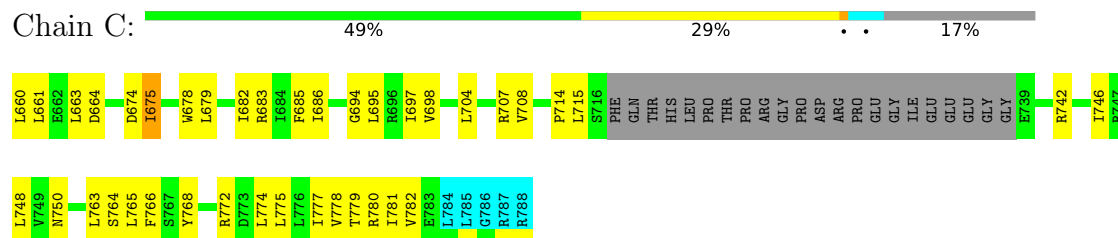
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

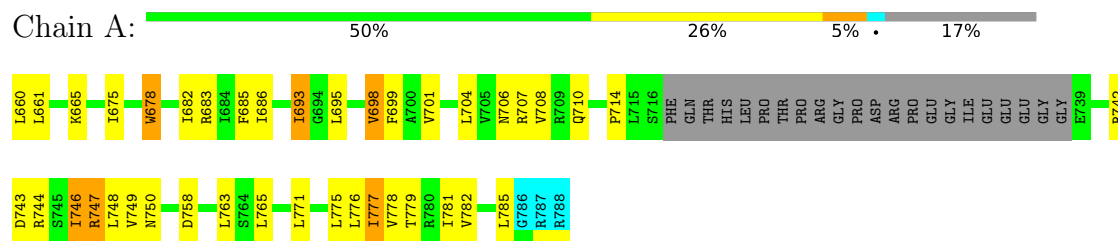


4.2 Scores per residue for each member of the ensemble

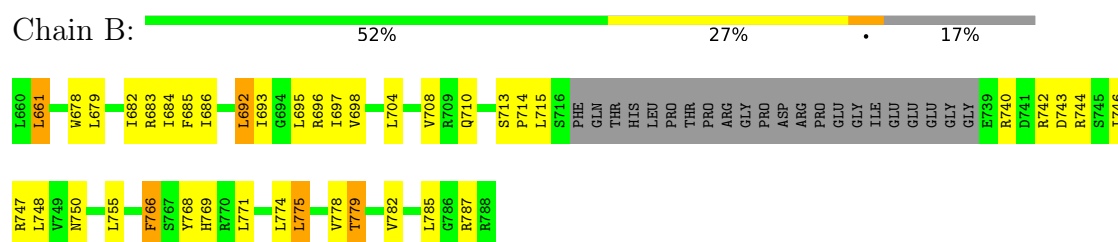
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

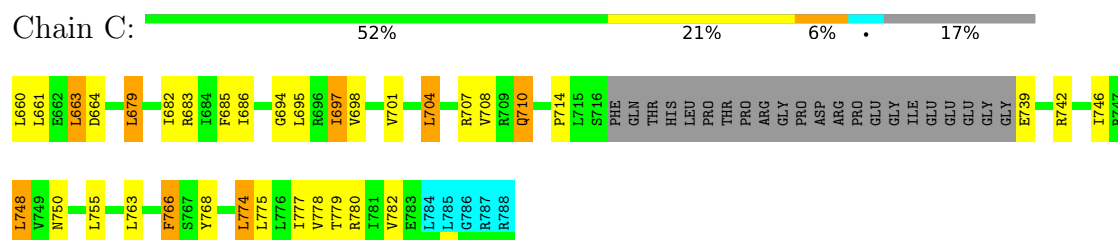
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

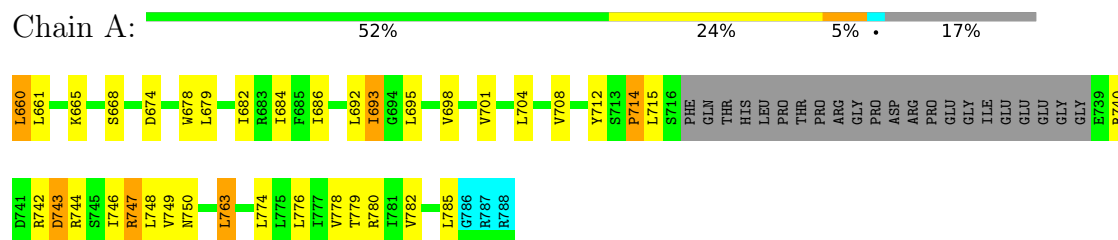


• Molecule 1: Envelope glycoprotein GP41



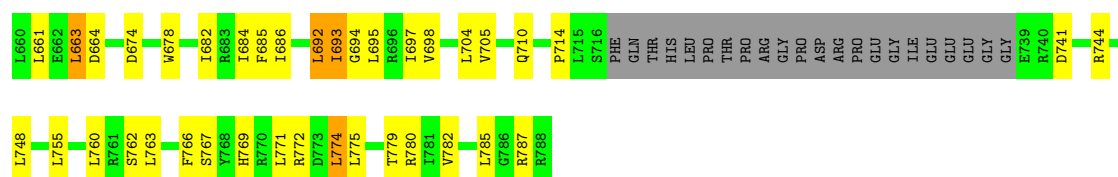
4.2.2 Score per residue for model 2

• Molecule 1: Envelope glycoprotein GP41



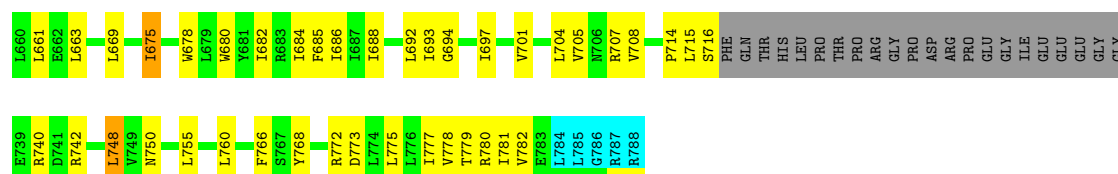
• Molecule 1: Envelope glycoprotein GP41





• Molecule 1: Envelope glycoprotein GP41

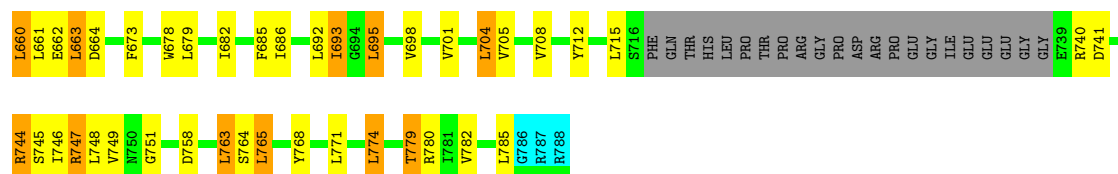
Chain C: 48% 29% 17%



4.2.3 Score per residue for model 3

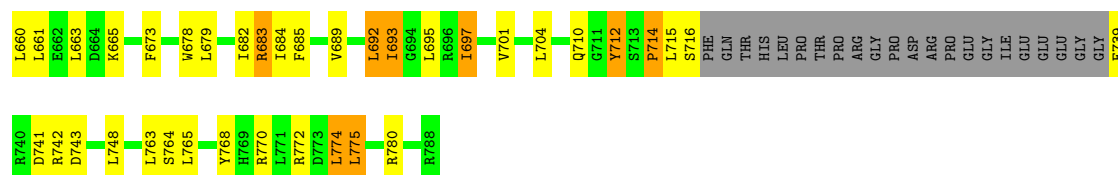
• Molecule 1: Envelope glycoprotein GP41

Chain A: 49% 23% 9% 17%



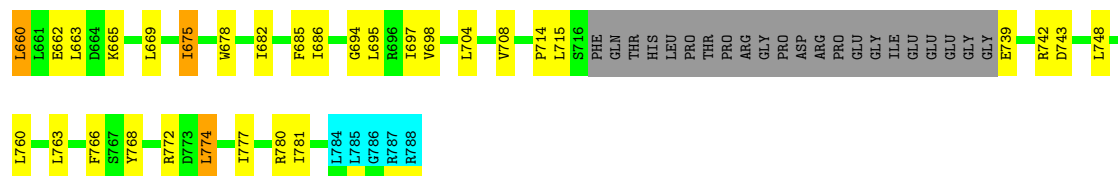
• Molecule 1: Envelope glycoprotein GP41

Chain B: 54% 22% 6% 17%



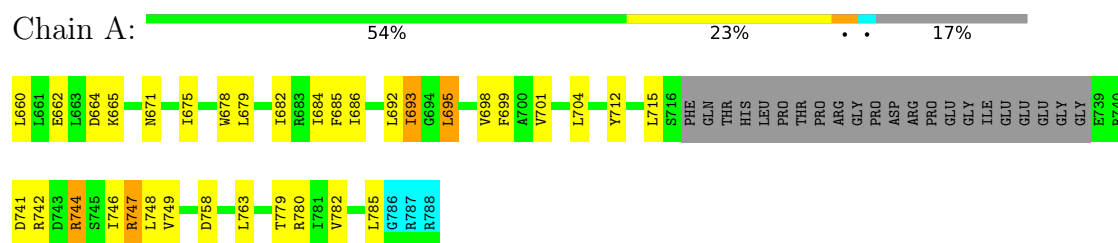
• Molecule 1: Envelope glycoprotein GP41

Chain C: 55% 22% 17%

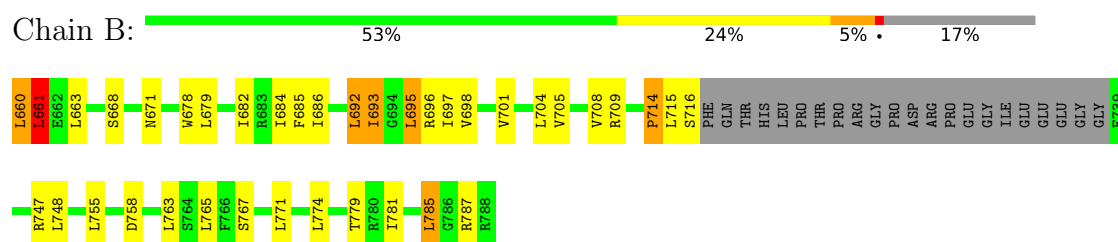


4.2.4 Score per residue for model 4

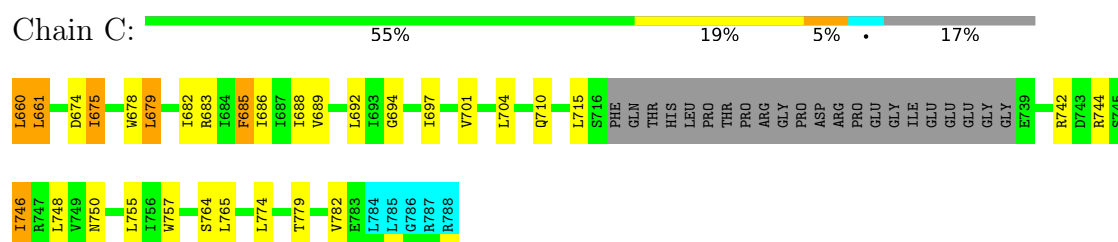
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

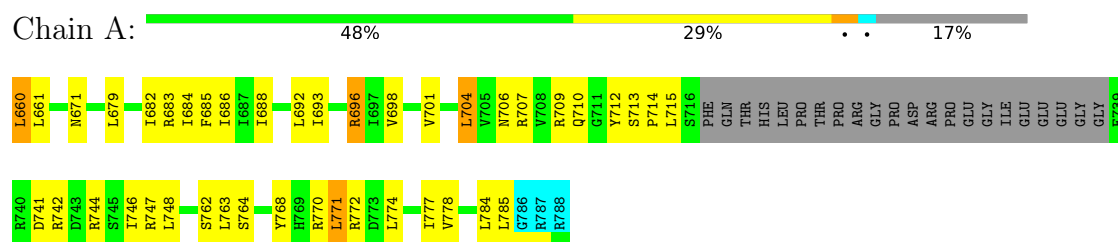


• Molecule 1: Envelope glycoprotein GP41



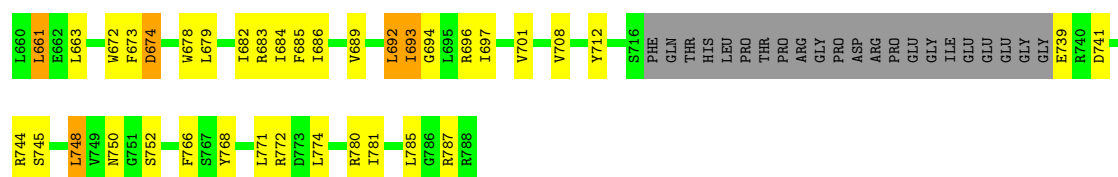
4.2.5 Score per residue for model 5

• Molecule 1: Envelope glycoprotein GP41



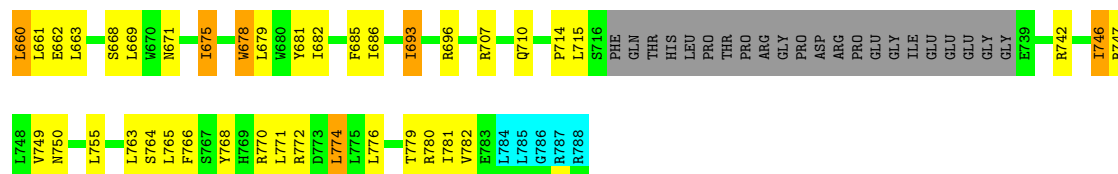
• Molecule 1: Envelope glycoprotein GP41





• Molecule 1: Envelope glycoprotein GP41

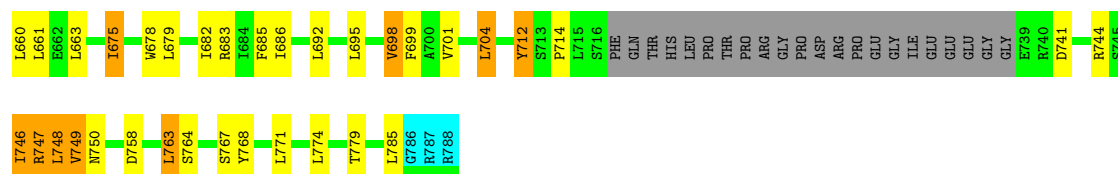
Chain C: 48% 26% 5% 17%



4.2.6 Score per residue for model 6

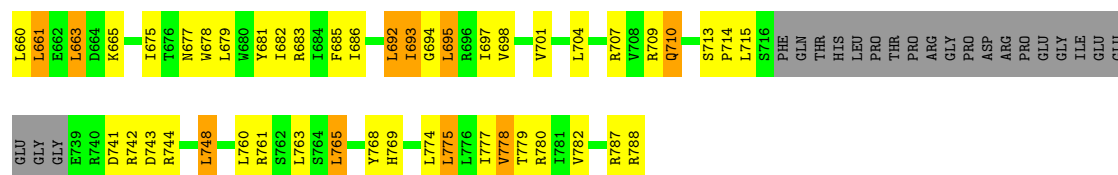
• Molecule 1: Envelope glycoprotein GP41

Chain A: 54% 19% 7% 17%



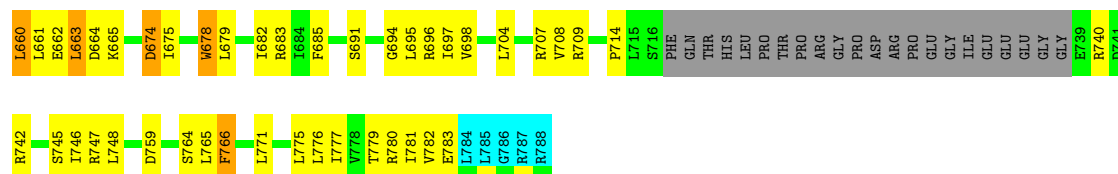
• Molecule 1: Envelope glycoprotein GP41

Chain B: 47% 29% 8% 17%



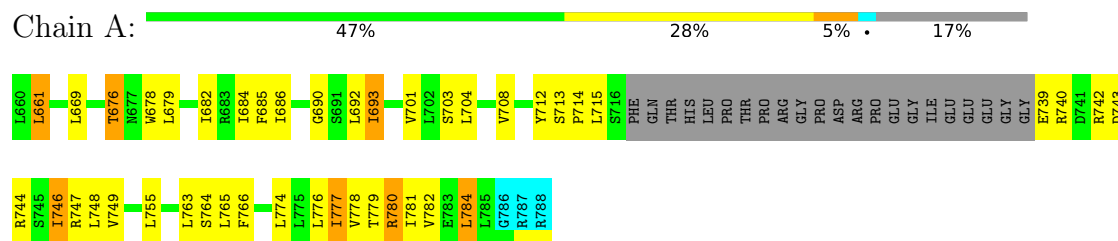
• Molecule 1: Envelope glycoprotein GP41

Chain C: 46% 29% 17%

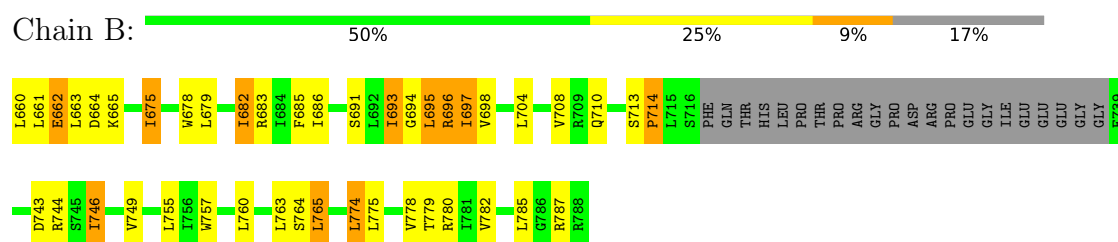


4.2.7 Score per residue for model 7

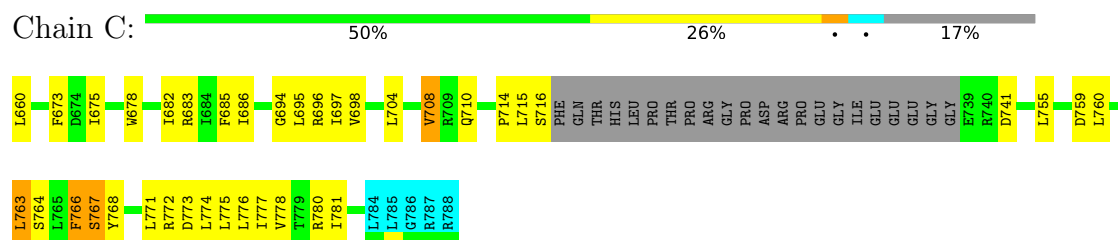
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41



4.2.8 Score per residue for model 8

• Molecule 1: Envelope glycoprotein GP41

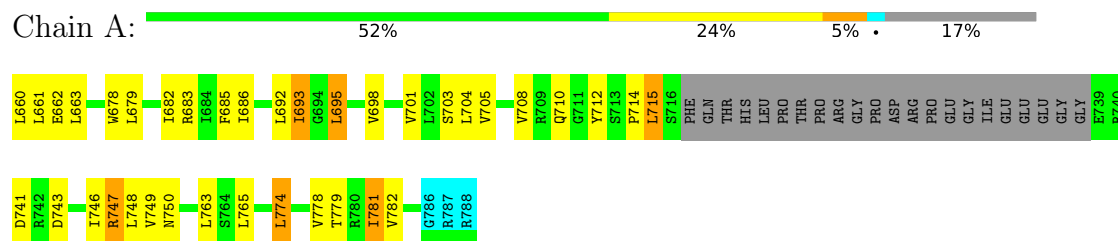


• Molecule 1: Envelope glycoprotein GP41

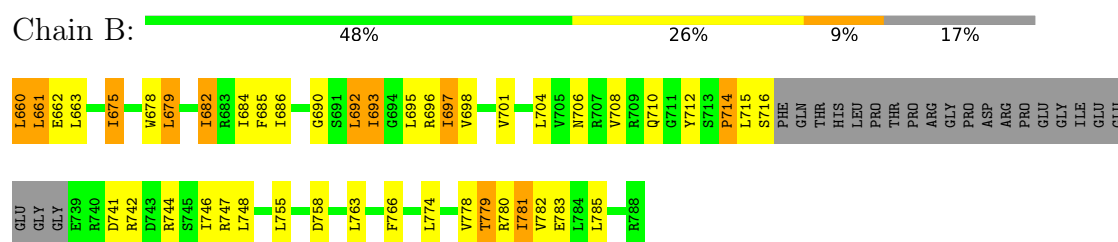


4.2.10 Score per residue for model 10

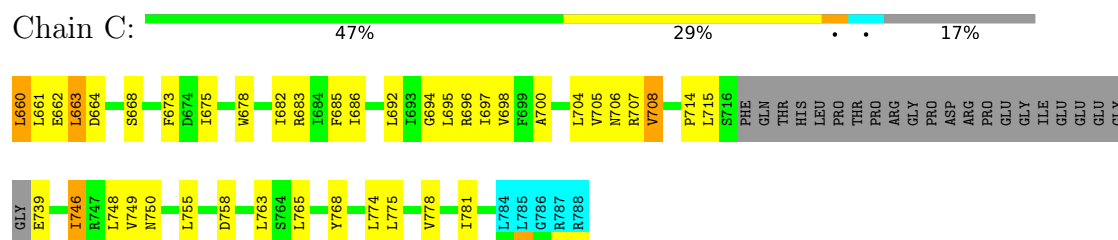
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

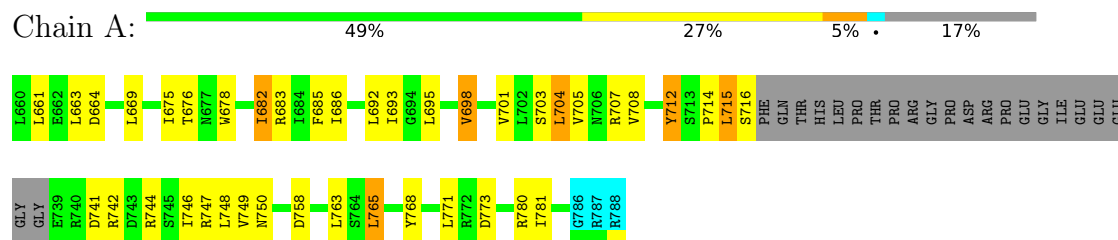


• Molecule 1: Envelope glycoprotein GP41



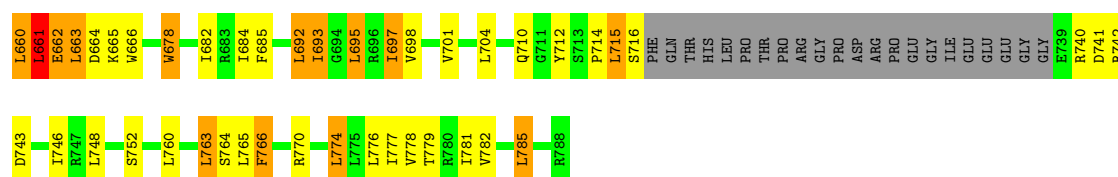
4.2.11 Score per residue for model 11

• Molecule 1: Envelope glycoprotein GP41



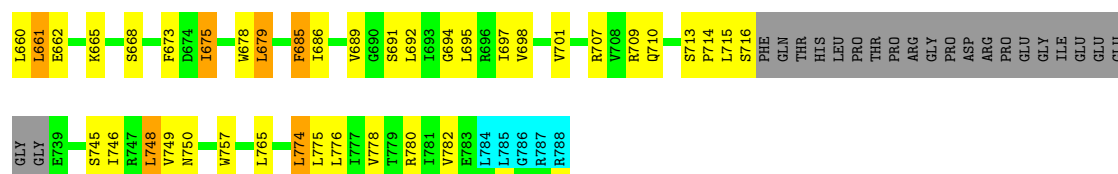
• Molecule 1: Envelope glycoprotein GP41





• Molecule 1: Envelope glycoprotein GP41

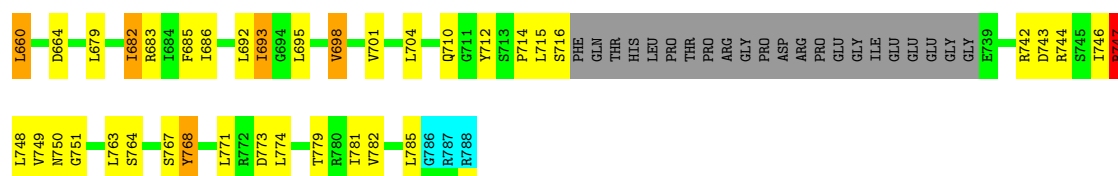
Chain C: 49% 26% 5% 17%



4.2.12 Score per residue for model 12

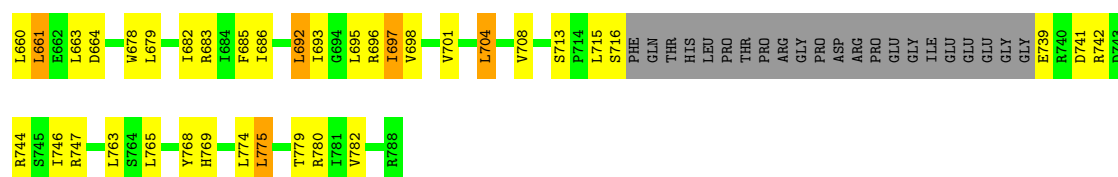
• Molecule 1: Envelope glycoprotein GP41

Chain A: 51% 25% 17%



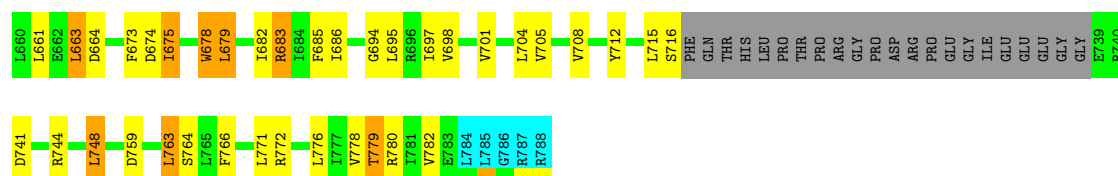
• Molecule 1: Envelope glycoprotein GP41

Chain B: 54% 25% 17%



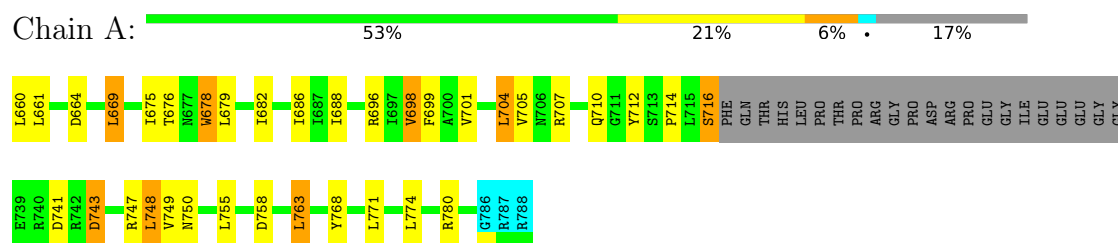
• Molecule 1: Envelope glycoprotein GP41

Chain C: 50% 22% 6% 17%

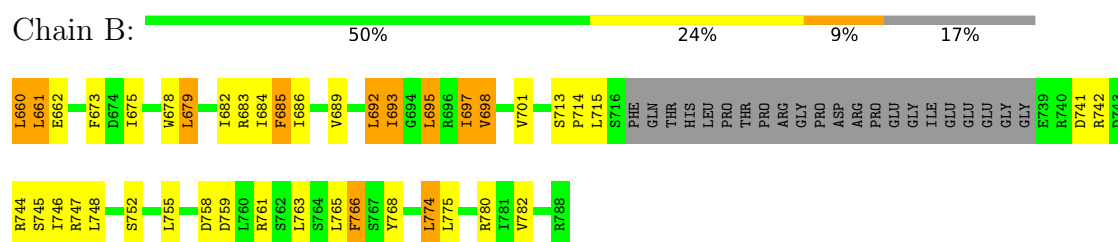


4.2.13 Score per residue for model 13

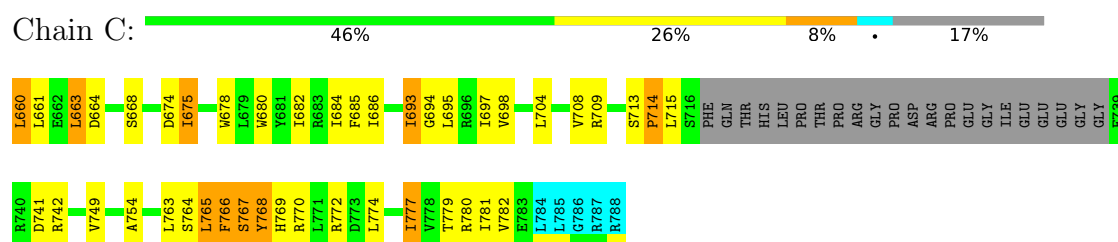
• Molecule 1: Envelope glycoprotein GP41



• Molecule 1: Envelope glycoprotein GP41

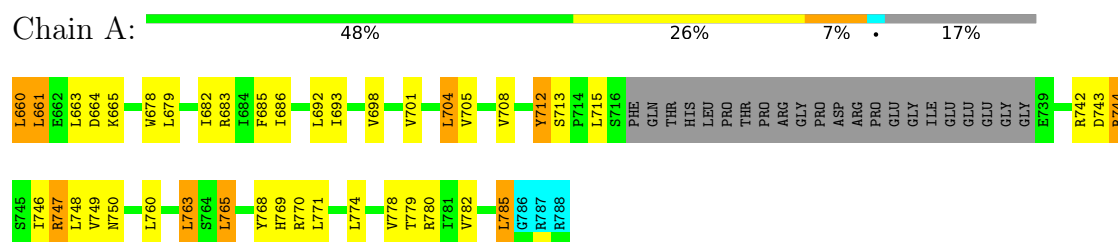


• Molecule 1: Envelope glycoprotein GP41



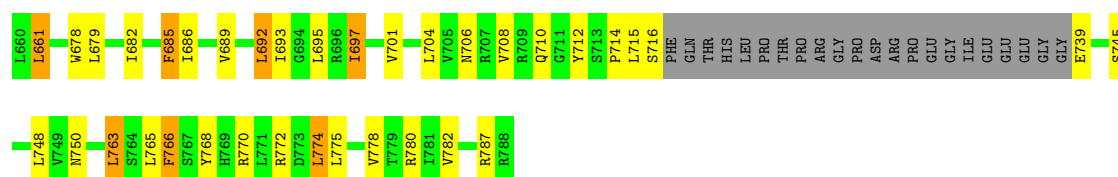
4.2.14 Score per residue for model 14

• Molecule 1: Envelope glycoprotein GP41



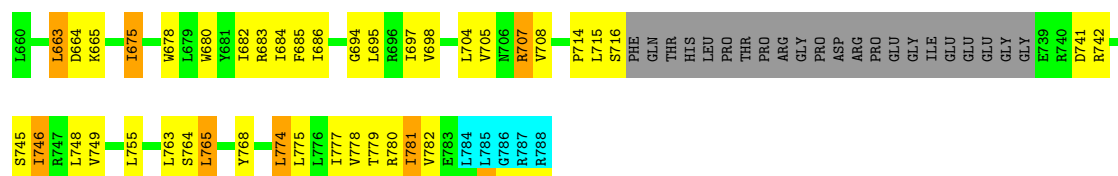
• Molecule 1: Envelope glycoprotein GP41





• Molecule 1: Envelope glycoprotein GP41

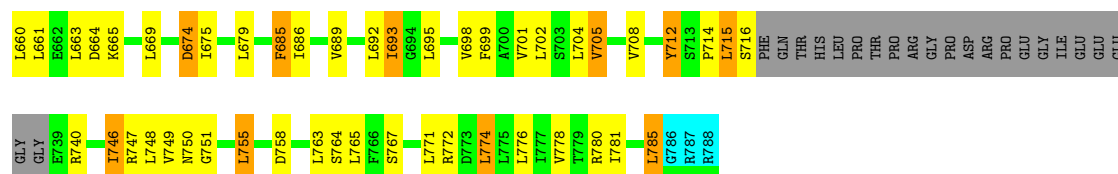
Chain C: 47% 26% 5% 17%



4.2.15 Score per residue for model 15

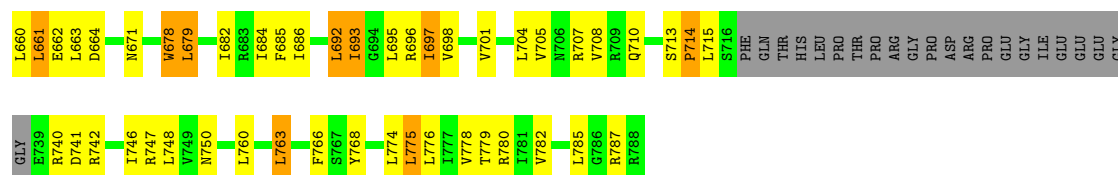
• Molecule 1: Envelope glycoprotein GP41

Chain A: 44% 29% 8% 17%



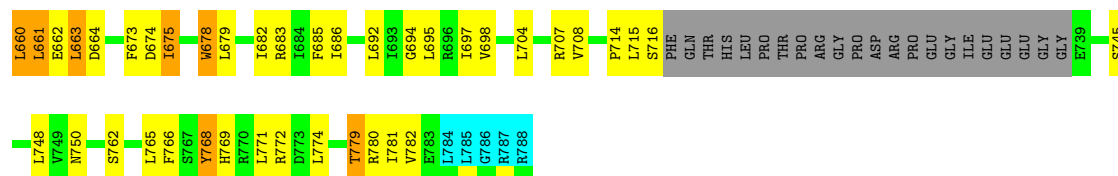
• Molecule 1: Envelope glycoprotein GP41

Chain B: 47% 29% 7% 17%



• Molecule 1: Envelope glycoprotein GP41

Chain C: 48% 26% 5% 17%



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	structure calculation	
X-PLOR NIH	refinement	

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	520
Number of shifts mapped to atoms	520
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	10%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (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	0.76±0.01	0±0/899 (0.0± 0.0%)	0.94±0.01	0±0/1223 (0.0± 0.0%)
1	B	0.75±0.01	0±0/925 (0.0± 0.0%)	0.92±0.01	0±0/1253 (0.0± 0.0%)
1	C	0.74±0.01	0±0/883 (0.0± 0.0%)	0.92±0.01	0±0/1201 (0.0± 0.0%)
All	All	0.75	0/40605 (0.0%)	0.93	1/55155 (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	A	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	681	TYR	CB-CG-CD1	-5.21	117.87	121.00	5	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	A	707	ARG	Sidechain	1
1	A	747	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	879	924	919	24±5
1	B	906	953	948	25±4
1	C	863	902	897	23±5
All	All	39720	41685	41460	861

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:781:ILE:HG23	1:B:746:ILE:HG23	0.86	1.47	8	1
1:A:686:ILE:HD12	1:C:686:ILE:HG21	0.81	1.52	9	12
1:A:705:VAL:HG22	1:A:748:LEU:HD11	0.80	1.53	13	1
1:B:781:ILE:HG23	1:C:746:ILE:HG23	0.79	1.52	4	2
1:A:686:ILE:HG21	1:B:686:ILE:HD12	0.78	1.55	15	12
1:A:774:LEU:HD22	1:A:777:ILE:HD11	0.77	1.55	8	1
1:B:785:LEU:HD23	1:C:750:ASN:ND2	0.75	1.96	9	4
1:A:779:THR:O	1:A:782:VAL:HG22	0.74	1.81	7	9
1:C:779:THR:O	1:C:782:VAL:HG22	0.73	1.83	8	10
1:A:748:LEU:O	1:A:748:LEU:HD13	0.73	1.84	5	8
1:A:669:LEU:HD23	1:A:676:THR:HG23	0.73	1.59	7	2
1:A:705:VAL:HG22	1:A:748:LEU:HD12	0.73	1.59	9	4
1:B:779:THR:O	1:B:782:VAL:HG22	0.71	1.85	9	10
1:A:758:ASP:OD1	1:B:715:LEU:HD22	0.71	1.86	15	2
1:C:759:ASP:O	1:C:763:LEU:HD22	0.71	1.85	7	1
1:B:742:ARG:O	1:B:746:ILE:HD12	0.71	1.85	12	1
1:A:746:ILE:HG22	1:C:781:ILE:HG21	0.70	1.62	14	1
1:A:698:VAL:O	1:A:701:VAL:HG22	0.70	1.86	12	14
1:B:682:ILE:HD12	1:B:683:ARG:N	0.69	2.02	1	6
1:A:678:TRP:O	1:A:682:ILE:HG23	0.69	1.86	6	11
1:A:777:ILE:HD13	1:A:778:VAL:N	0.68	2.02	7	2
1:A:746:ILE:O	1:A:749:VAL:HG22	0.68	1.88	11	1
1:A:663:LEU:HD23	1:B:660:LEU:N	0.68	2.03	8	1
1:A:693:ILE:O	1:A:693:ILE:HD13	0.68	1.89	15	2
1:A:768:TYR:CE1	1:A:771:LEU:HD23	0.68	2.23	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:781:ILE:HG21	1:B:746:ILE:CG2	0.68	2.19	10	2
1:A:705:VAL:HG22	1:A:748:LEU:HD23	0.68	1.64	3	1
1:C:775:LEU:O	1:C:778:VAL:HG22	0.68	1.88	7	4
1:B:663:LEU:HD12	1:C:660:LEU:HD23	0.67	1.66	3	1
1:C:682:ILE:HD12	1:C:683:ARG:N	0.67	2.05	14	9
1:C:675:ILE:O	1:C:675:ILE:HD13	0.67	1.90	9	10
1:A:682:ILE:HD12	1:A:683:ARG:N	0.67	2.04	14	5
1:C:742:ARG:O	1:C:746:ILE:HD12	0.67	1.90	14	5
1:A:705:VAL:HG23	1:A:748:LEU:HD12	0.66	1.66	15	1
1:A:778:VAL:O	1:A:781:ILE:HG22	0.66	1.90	10	2
1:B:686:ILE:HG21	1:C:686:ILE:HD12	0.66	1.67	7	9
1:B:781:ILE:HG23	1:C:746:ILE:CG2	0.66	2.21	4	1
1:A:705:VAL:CG2	1:A:748:LEU:HD12	0.66	2.21	14	3
1:C:748:LEU:HD13	1:C:749:VAL:N	0.65	2.07	11	1
1:B:678:TRP:O	1:B:682:ILE:HG23	0.65	1.91	9	14
1:C:771:LEU:O	1:C:771:LEU:HD23	0.65	1.92	15	1
1:B:697:ILE:O	1:B:697:ILE:HD13	0.64	1.92	10	7
1:C:697:ILE:HD13	1:C:697:ILE:O	0.64	1.92	1	1
1:B:763:LEU:HA	1:B:774:LEU:HD22	0.64	1.69	3	1
1:B:778:VAL:O	1:B:781:ILE:HG22	0.64	1.91	10	1
1:B:771:LEU:HD23	1:B:771:LEU:O	0.64	1.93	2	2
1:A:660:LEU:N	1:C:663:LEU:HD23	0.63	2.08	15	8
1:A:746:ILE:HB	1:C:781:ILE:HG21	0.63	1.71	10	3
1:A:763:LEU:O	1:A:774:LEU:HD13	0.63	1.93	10	1
1:B:693:ILE:HD11	1:C:696:ARG:NE	0.63	2.07	7	3
1:B:675:ILE:HD13	1:B:675:ILE:O	0.62	1.95	7	1
1:A:693:ILE:HD11	1:B:696:ARG:HE	0.62	1.53	12	3
1:A:743:ASP:HA	1:C:781:ILE:HD11	0.62	1.72	14	1
1:C:774:LEU:HD22	1:C:777:ILE:HD12	0.62	1.72	14	1
1:B:693:ILE:HD11	1:C:696:ARG:HE	0.62	1.52	10	2
1:C:745:SER:O	1:C:748:LEU:HD12	0.61	1.95	11	1
1:C:777:ILE:HG22	1:C:781:ILE:HD11	0.61	1.70	6	2
1:C:694:GLY:O	1:C:697:ILE:HG22	0.61	1.95	9	13
1:C:759:ASP:O	1:C:763:LEU:HD12	0.61	1.96	12	1
1:A:781:ILE:HD11	1:B:746:ILE:CG2	0.61	2.25	11	1
1:C:705:VAL:HG13	1:C:748:LEU:HD21	0.61	1.72	12	2
1:A:758:ASP:OD2	1:B:715:LEU:HD22	0.61	1.95	13	2
1:A:758:ASP:CG	1:B:715:LEU:HD13	0.61	2.16	6	1
1:C:778:VAL:O	1:C:781:ILE:HG22	0.61	1.94	14	2
1:C:678:TRP:O	1:C:682:ILE:HG23	0.60	1.96	15	12
1:B:781:ILE:HD12	1:C:746:ILE:HG13	0.60	1.72	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:774:LEU:O	1:B:778:VAL:HG23	0.60	1.97	11	4
1:A:780:ARG:NH2	1:A:784:LEU:HD21	0.60	2.12	7	1
1:B:694:GLY:O	1:B:697:ILE:HD12	0.60	1.97	7	1
1:A:777:ILE:HD12	1:A:778:VAL:N	0.59	2.12	5	1
1:B:775:LEU:HD13	1:B:775:LEU:O	0.59	1.97	6	10
1:A:746:ILE:CG2	1:C:781:ILE:HG21	0.59	2.27	14	1
1:C:777:ILE:HG22	1:C:781:ILE:CD1	0.59	2.27	6	2
1:A:693:ILE:HD12	1:A:693:ILE:O	0.59	1.97	8	4
1:C:663:LEU:HD22	1:C:663:LEU:O	0.59	1.96	14	4
1:B:693:ILE:HD11	1:C:696:ARG:HG3	0.59	1.75	5	1
1:A:774:LEU:HD12	1:B:742:ARG:NE	0.59	2.13	9	2
1:B:763:LEU:O	1:B:774:LEU:HD13	0.59	1.97	14	3
1:B:763:LEU:O	1:B:774:LEU:HD22	0.59	1.97	11	2
1:A:755:LEU:HD22	1:A:755:LEU:O	0.59	1.97	15	1
1:A:704:LEU:HD23	1:A:707:ARG:HD2	0.59	1.75	8	1
1:C:663:LEU:HD13	1:C:664:ASP:N	0.58	2.13	1	8
1:B:660:LEU:C	1:B:661:LEU:HD22	0.58	2.19	11	2
1:C:774:LEU:HD13	1:C:774:LEU:O	0.58	1.99	10	4
1:C:763:LEU:HD13	1:C:764:SER:H	0.58	1.57	12	1
1:B:686:ILE:CG2	1:C:686:ILE:HD12	0.57	2.28	7	9
1:C:660:LEU:N	1:C:660:LEU:HD13	0.57	2.14	4	2
1:A:675:ILE:HD13	1:A:675:ILE:O	0.57	1.99	8	2
1:C:675:ILE:HD13	1:C:678:TRP:CZ3	0.57	2.33	8	1
1:C:768:TYR:O	1:C:770:ARG:N	0.57	2.37	13	1
1:B:710:GLN:O	1:B:715:LEU:HD11	0.57	1.98	15	1
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.57	1.76	10	4
1:A:742:ARG:O	1:A:746:ILE:HD12	0.57	1.99	1	4
1:B:785:LEU:HD23	1:C:750:ASN:HD22	0.57	1.57	5	2
1:C:675:ILE:HD12	1:C:678:TRP:CE3	0.57	2.35	7	1
1:A:704:LEU:HD22	1:B:712:TYR:O	0.57	1.99	8	1
1:B:781:ILE:O	1:B:785:LEU:HD12	0.57	1.99	4	1
1:B:715:LEU:O	1:B:715:LEU:HD23	0.56	2.00	15	4
1:C:763:LEU:HD23	1:C:764:SER:H	0.56	1.60	7	1
1:A:763:LEU:HA	1:A:774:LEU:HD22	0.56	1.77	3	3
1:B:781:ILE:HG21	1:C:746:ILE:CG2	0.56	2.31	11	2
1:A:749:VAL:HG23	1:A:750:ASN:ND2	0.56	2.15	11	1
1:B:785:LEU:HD23	1:C:750:ASN:HB2	0.56	1.75	1	1
1:A:663:LEU:HD12	1:B:660:LEU:N	0.56	2.15	9	4
1:A:746:ILE:HD12	1:C:781:ILE:CD1	0.56	2.30	5	1
1:A:749:VAL:HG21	1:C:782:VAL:HG12	0.56	1.77	11	1
1:C:685:PHE:O	1:C:689:VAL:HG23	0.56	2.01	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:701:VAL:O	1:A:705:VAL:HG23	0.56	2.01	13	2
1:C:698:VAL:O	1:C:701:VAL:HG22	0.56	2.01	11	1
1:B:785:LEU:HD13	1:C:750:ASN:HD21	0.56	1.61	4	1
1:C:763:LEU:HD23	1:C:764:SER:N	0.56	2.15	7	1
1:A:682:ILE:HD12	1:A:683:ARG:H	0.55	1.62	5	4
1:C:693:ILE:HD12	1:C:693:ILE:O	0.55	2.01	5	1
1:B:758:ASP:CG	1:C:715:LEU:HD22	0.55	2.21	13	1
1:C:764:SER:HB3	1:C:771:LEU:HD12	0.55	1.78	7	1
1:A:763:LEU:O	1:A:774:LEU:HD22	0.55	2.01	13	1
1:A:715:LEU:HD23	1:C:758:ASP:OD2	0.55	2.01	10	1
1:B:785:LEU:HD23	1:C:750:ASN:CG	0.55	2.22	10	1
1:A:705:VAL:HG22	1:A:748:LEU:CD1	0.55	2.29	13	1
1:A:748:LEU:O	1:A:748:LEU:HD22	0.55	2.01	13	1
1:C:695:LEU:O	1:C:698:VAL:HG12	0.55	2.00	15	11
1:B:710:GLN:O	1:B:715:LEU:HD12	0.55	2.01	14	3
1:C:763:LEU:C	1:C:763:LEU:HD22	0.55	2.22	12	1
1:B:692:LEU:HD12	1:B:693:ILE:N	0.55	2.17	3	12
1:B:693:ILE:HD12	1:B:693:ILE:O	0.54	2.02	10	2
1:A:704:LEU:HD11	1:B:712:TYR:O	0.54	2.03	14	4
1:C:763:LEU:HD13	1:C:764:SER:N	0.54	2.17	12	1
1:A:780:ARG:NH2	1:A:784:LEU:HD11	0.54	2.18	7	1
1:B:697:ILE:HD13	1:B:698:VAL:H	0.54	1.63	7	1
1:B:774:LEU:HD11	1:C:742:ARG:CZ	0.54	2.32	13	1
1:A:749:VAL:HG12	1:A:750:ASN:ND2	0.54	2.18	12	8
1:A:747:ARG:NE	1:C:782:VAL:HA	0.54	2.18	2	1
1:A:746:ILE:HD12	1:C:781:ILE:HD12	0.54	1.78	5	1
1:A:746:ILE:HG22	1:C:781:ILE:HD13	0.54	1.79	8	1
1:B:663:LEU:CD1	1:C:660:LEU:HD22	0.54	2.32	7	2
1:C:777:ILE:HG22	1:C:781:ILE:HD12	0.54	1.78	14	1
1:A:763:LEU:HA	1:A:774:LEU:HD13	0.53	1.78	12	4
1:A:774:LEU:HD11	1:B:742:ARG:NH2	0.53	2.18	3	1
1:B:785:LEU:HD22	1:C:750:ASN:ND2	0.53	2.18	4	2
1:A:781:ILE:HG21	1:B:746:ILE:HG21	0.53	1.80	10	2
1:A:774:LEU:CD1	1:A:777:ILE:HD11	0.53	2.34	5	1
1:B:695:LEU:O	1:B:698:VAL:HG12	0.53	2.02	1	9
1:A:748:LEU:HD23	1:A:748:LEU:O	0.53	2.04	8	1
1:A:696:ARG:HE	1:C:693:ILE:HD11	0.53	1.63	5	1
1:C:773:ASP:OD2	1:C:774:LEU:HD22	0.53	2.04	7	1
1:B:781:ILE:HG21	1:C:746:ILE:HG22	0.53	1.79	11	1
1:C:748:LEU:C	1:C:748:LEU:HD22	0.53	2.24	11	1
1:B:705:VAL:HG13	1:B:748:LEU:CD2	0.53	2.34	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:785:LEU:HD22	1:B:750:ASN:ND2	0.52	2.19	9	3
1:A:774:LEU:HD13	1:A:774:LEU:O	0.52	2.05	8	1
1:A:781:ILE:HD11	1:B:746:ILE:HB	0.52	1.80	11	1
1:A:774:LEU:O	1:A:778:VAL:HG23	0.52	2.04	14	2
1:B:705:VAL:HG22	1:B:748:LEU:HD23	0.52	1.80	15	1
1:B:661:LEU:N	1:B:661:LEU:HD22	0.52	2.20	10	10
1:A:758:ASP:CB	1:B:715:LEU:HD13	0.52	2.34	6	2
1:B:708:VAL:HG11	1:B:748:LEU:HD21	0.52	1.82	14	1
1:A:763:LEU:HD23	1:A:771:LEU:HD11	0.52	1.80	5	2
1:A:675:ILE:CG1	1:A:679:LEU:HD23	0.52	2.35	13	1
1:C:693:ILE:C	1:C:693:ILE:HD13	0.52	2.25	13	1
1:B:708:VAL:HG11	1:B:748:LEU:HD11	0.52	1.82	5	1
1:C:745:SER:O	1:C:748:LEU:HD22	0.52	2.05	8	1
1:B:785:LEU:HD22	1:C:747:ARG:HA	0.52	1.81	9	1
1:A:774:LEU:O	1:A:778:VAL:HG13	0.51	2.05	2	1
1:B:660:LEU:HG	1:B:661:LEU:HD22	0.51	1.82	6	1
1:A:781:ILE:CD1	1:B:746:ILE:HD13	0.51	2.35	12	1
1:A:785:LEU:HD23	1:B:750:ASN:ND2	0.51	2.21	8	3
1:B:748:LEU:O	1:B:748:LEU:HD23	0.51	2.05	6	1
1:C:748:LEU:HD12	1:C:748:LEU:O	0.51	2.05	12	1
1:A:748:LEU:C	1:A:748:LEU:HD13	0.51	2.26	13	1
1:C:777:ILE:O	1:C:781:ILE:HG13	0.51	2.05	2	1
1:B:663:LEU:HD13	1:C:660:LEU:HD22	0.51	1.83	10	2
1:C:749:VAL:HG12	1:C:750:ASN:ND2	0.51	2.21	9	1
1:B:693:ILE:C	1:B:693:ILE:HD13	0.51	2.26	7	2
1:A:758:ASP:HB3	1:B:715:LEU:HD13	0.51	1.82	15	1
1:C:774:LEU:HD22	1:C:777:ILE:CD1	0.50	2.36	14	1
1:A:777:ILE:HD11	1:B:742:ARG:HH11	0.50	1.66	1	1
1:B:715:LEU:O	1:B:716:SER:C	0.50	2.49	8	7
1:A:774:LEU:HD12	1:A:777:ILE:HD11	0.50	1.81	5	1
1:B:785:LEU:HD22	1:C:750:ASN:CG	0.50	2.27	4	1
1:C:715:LEU:O	1:C:716:SER:C	0.50	2.50	7	5
1:A:748:LEU:HD13	1:B:714:PRO:CG	0.50	2.37	4	1
1:A:669:LEU:CD2	1:A:676:THR:HG23	0.50	2.34	7	1
1:A:696:ARG:HG3	1:C:693:ILE:HD11	0.50	1.82	13	1
1:A:693:ILE:HD13	1:A:693:ILE:C	0.49	2.27	1	2
1:C:748:LEU:O	1:C:748:LEU:HD23	0.49	2.06	15	2
1:B:675:ILE:HG13	1:B:679:LEU:HD23	0.49	1.84	6	1
1:B:785:LEU:HD13	1:C:750:ASN:ND2	0.49	2.23	4	1
1:A:749:VAL:HG23	1:A:750:ASN:HD22	0.49	1.66	11	1
1:C:774:LEU:HD13	1:C:777:ILE:HG22	0.49	1.85	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:781:ILE:HG21	1:B:746:ILE:HG23	0.49	1.84	10	2
1:A:746:ILE:HG12	1:C:778:VAL:HG12	0.49	1.85	12	2
1:A:704:LEU:HD22	1:B:707:ARG:NH2	0.49	2.23	6	1
1:A:784:LEU:N	1:A:784:LEU:HD13	0.49	2.23	7	1
1:A:742:ARG:CZ	1:C:774:LEU:HD21	0.49	2.38	11	1
1:A:705:VAL:HG23	1:A:748:LEU:CB	0.49	2.38	8	1
1:A:695:LEU:HD23	1:A:695:LEU:O	0.49	2.07	2	1
1:C:660:LEU:HD22	1:C:660:LEU:C	0.49	2.27	3	1
1:A:771:LEU:O	1:A:771:LEU:HD12	0.49	2.08	8	1
1:A:781:ILE:HD11	1:B:746:ILE:CB	0.49	2.37	11	1
1:A:690:GLY:O	1:A:693:ILE:HG23	0.49	2.07	7	1
1:B:697:ILE:HD13	1:B:698:VAL:N	0.49	2.23	7	1
1:B:694:GLY:O	1:B:697:ILE:HG22	0.48	2.08	2	3
1:C:708:VAL:HG12	1:C:748:LEU:HD11	0.48	1.85	10	1
1:A:748:LEU:HD13	1:B:714:PRO:HG3	0.48	1.83	4	2
1:B:705:VAL:HG22	1:B:748:LEU:HD13	0.48	1.85	4	1
1:B:781:ILE:CG2	1:C:746:ILE:HG23	0.48	2.39	5	1
1:B:777:ILE:HD12	1:B:778:VAL:N	0.48	2.23	6	1
1:A:743:ASP:O	1:C:781:ILE:HG23	0.48	2.09	10	2
1:A:716:SER:HA	1:C:754:ALA:HB1	0.48	1.84	13	1
1:A:746:ILE:CG2	1:C:781:ILE:HD12	0.48	2.38	2	1
1:B:764:SER:C	1:B:765:LEU:HD12	0.48	2.29	3	1
1:C:679:LEU:HD13	1:C:679:LEU:O	0.48	2.09	4	2
1:B:661:LEU:HD12	1:B:666:TRP:CE2	0.48	2.44	11	1
1:A:675:ILE:HG12	1:A:679:LEU:HD23	0.48	1.84	13	1
1:B:675:ILE:HD11	1:B:678:TRP:CE3	0.48	2.43	7	1
1:A:675:ILE:HG13	1:A:679:LEU:HD23	0.48	1.84	15	2
1:A:747:ARG:NH1	1:C:781:ILE:HG22	0.48	2.24	5	1
1:B:679:LEU:HD13	1:B:679:LEU:O	0.48	2.08	10	3
1:A:743:ASP:O	1:C:781:ILE:HG21	0.47	2.09	2	1
1:A:743:ASP:CB	1:C:781:ILE:HD12	0.47	2.38	13	1
1:A:780:ARG:HH21	1:A:784:LEU:HD21	0.47	1.69	7	1
1:C:764:SER:CB	1:C:771:LEU:HD12	0.47	2.39	9	2
1:C:765:LEU:N	1:C:765:LEU:HD22	0.47	2.24	8	1
1:A:748:LEU:HD22	1:A:751:GLY:HA3	0.47	1.85	15	2
1:B:692:LEU:HD12	1:B:693:ILE:H	0.47	1.70	6	10
1:B:755:LEU:HD21	1:C:710:GLN:NE2	0.47	2.25	4	1
1:B:765:LEU:HD13	1:B:765:LEU:O	0.47	2.09	8	1
1:A:746:ILE:HG21	1:C:781:ILE:HD12	0.47	1.85	2	1
1:A:774:LEU:HD11	1:B:742:ARG:CZ	0.47	2.40	3	1
1:A:705:VAL:HG23	1:A:748:LEU:CD1	0.47	2.39	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:774:LEU:HD12	1:C:742:ARG:HE	0.47	1.68	9	1
1:B:689:VAL:O	1:B:692:LEU:HD11	0.47	2.10	8	1
1:C:748:LEU:HD22	1:C:748:LEU:O	0.47	2.10	11	1
1:A:746:ILE:O	1:A:749:VAL:HB	0.47	2.10	6	4
1:A:715:LEU:H	1:A:715:LEU:HD23	0.47	1.69	7	2
1:B:675:ILE:HD11	1:B:679:LEU:HD23	0.47	1.86	10	1
1:B:776:LEU:O	1:B:779:THR:HG22	0.47	2.09	15	2
1:A:774:LEU:HD12	1:B:742:ARG:HE	0.47	1.70	9	1
1:A:774:LEU:HD13	1:A:774:LEU:C	0.47	2.31	7	1
1:B:669:LEU:HD12	1:B:675:ILE:CG2	0.47	2.40	8	1
1:B:690:GLY:O	1:B:693:ILE:HG23	0.47	2.09	10	1
1:C:695:LEU:O	1:C:695:LEU:HD23	0.47	2.10	11	1
1:A:776:LEU:O	1:A:779:THR:HG22	0.47	2.10	2	1
1:A:748:LEU:HD21	1:B:714:PRO:CG	0.46	2.40	7	1
1:A:746:ILE:HD13	1:C:781:ILE:CD1	0.46	2.40	15	1
1:C:777:ILE:CG2	1:C:781:ILE:HD11	0.46	2.40	6	2
1:A:713:SER:OG	1:C:708:VAL:HG23	0.46	2.09	7	1
1:B:675:ILE:HD12	1:B:675:ILE:O	0.46	2.10	10	1
1:A:707:ARG:HH21	1:A:708:VAL:HG23	0.46	1.70	1	1
1:A:747:ARG:C	1:A:749:VAL:N	0.46	2.69	7	7
1:C:661:LEU:HD12	1:C:661:LEU:N	0.46	2.25	15	3
1:C:660:LEU:C	1:C:660:LEU:HD12	0.46	2.31	9	2
1:A:703:SER:OG	1:C:700:ALA:HB1	0.46	2.09	10	1
1:C:755:LEU:C	1:C:755:LEU:HD13	0.46	2.31	10	2
1:B:708:VAL:CG1	1:B:748:LEU:HD11	0.46	2.41	8	1
1:A:693:ILE:C	1:A:693:ILE:HD13	0.46	2.30	10	1
1:A:693:ILE:HG22	1:C:693:ILE:HG21	0.46	1.86	2	1
1:C:708:VAL:CG1	1:C:748:LEU:HD11	0.46	2.40	10	1
1:C:755:LEU:C	1:C:755:LEU:HD23	0.46	2.31	5	5
1:A:747:ARG:HG3	1:A:747:ARG:O	0.46	2.11	7	1
1:C:778:VAL:O	1:C:782:VAL:HG13	0.46	2.10	11	1
1:B:763:LEU:HA	1:B:774:LEU:HD13	0.45	1.87	7	1
1:B:685:PHE:O	1:B:689:VAL:HG23	0.45	2.11	13	2
1:B:686:ILE:HG22	1:C:686:ILE:HD12	0.45	1.88	2	1
1:B:748:LEU:C	1:B:748:LEU:HD23	0.45	2.31	2	1
1:C:663:LEU:C	1:C:663:LEU:HD13	0.45	2.32	3	2
1:A:696:ARG:NE	1:C:693:ILE:HD11	0.45	2.26	5	1
1:A:746:ILE:O	1:A:749:VAL:HG23	0.45	2.12	12	2
1:B:708:VAL:CG1	1:B:748:LEU:HD12	0.45	2.41	1	1
1:A:693:ILE:HG13	1:B:693:ILE:HG22	0.45	1.89	3	2
1:C:774:LEU:C	1:C:774:LEU:HD13	0.45	2.32	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:705:VAL:HG22	1:B:748:LEU:HD11	0.45	1.88	2	1
1:B:663:LEU:CD1	1:C:660:LEU:HD23	0.45	2.39	3	1
1:A:686:ILE:CG2	1:B:686:ILE:HD12	0.45	2.37	7	1
1:A:715:LEU:HD23	1:A:716:SER:N	0.45	2.27	11	2
1:A:696:ARG:CG	1:C:693:ILE:HD11	0.45	2.42	13	1
1:C:663:LEU:HD22	1:C:663:LEU:C	0.45	2.32	14	1
1:A:706:ASN:O	1:A:710:GLN:HB2	0.45	2.12	5	2
1:B:755:LEU:C	1:B:755:LEU:HD23	0.45	2.31	1	2
1:A:743:ASP:HA	1:C:781:ILE:HD13	0.45	1.88	2	1
1:A:743:ASP:HB3	1:C:781:ILE:HD12	0.45	1.87	13	1
1:B:686:ILE:HG21	1:C:686:ILE:CD1	0.45	2.42	14	1
1:A:695:LEU:O	1:A:698:VAL:HG12	0.45	2.12	4	3
1:B:781:ILE:HG23	1:C:746:ILE:HG13	0.45	1.89	5	1
1:B:705:VAL:HA	1:B:748:LEU:HD13	0.45	1.88	8	1
1:A:781:ILE:CG2	1:B:746:ILE:HG23	0.45	2.42	7	1
1:A:747:ARG:NE	1:A:750:ASN:ND2	0.45	2.64	2	1
1:A:704:LEU:HD13	1:A:707:ARG:NH2	0.45	2.27	11	2
1:C:663:LEU:HD13	1:C:663:LEU:C	0.45	2.32	13	5
1:A:765:LEU:HD22	1:A:765:LEU:O	0.45	2.12	11	1
1:B:684:ILE:HD12	1:B:684:ILE:N	0.45	2.25	3	10
1:A:758:ASP:HB3	1:B:710:GLN:CB	0.45	2.42	3	1
1:A:693:ILE:HD11	1:B:696:ARG:HG2	0.45	1.88	7	1
1:B:669:LEU:HD12	1:B:675:ILE:HG21	0.45	1.89	8	1
1:C:777:ILE:O	1:C:781:ILE:HG12	0.45	2.12	13	1
1:B:663:LEU:CD1	1:C:660:LEU:HD13	0.45	2.42	15	1
1:A:669:LEU:HD22	1:A:676:THR:OG1	0.44	2.13	8	1
1:B:715:LEU:HD22	1:B:715:LEU:N	0.44	2.27	8	1
1:B:682:ILE:HD12	1:B:683:ARG:H	0.44	1.70	5	1
1:A:704:LEU:HD22	1:A:707:ARG:NH1	0.44	2.27	13	1
1:A:663:LEU:C	1:A:663:LEU:HD13	0.44	2.31	8	1
1:C:661:LEU:HD22	1:C:661:LEU:N	0.44	2.26	9	1
1:A:776:LEU:C	1:A:776:LEU:HD13	0.44	2.32	8	1
1:C:715:LEU:HD22	1:C:715:LEU:N	0.44	2.27	11	1
1:B:672:TRP:O	1:B:674:ASP:N	0.44	2.50	5	1
1:A:660:LEU:CB	1:C:663:LEU:HD21	0.44	2.42	3	1
1:A:705:VAL:HG23	1:A:748:LEU:HD13	0.44	1.90	8	1
1:B:765:LEU:HD13	1:B:765:LEU:C	0.44	2.33	8	1
1:A:748:LEU:HD23	1:B:714:PRO:HB3	0.44	1.90	9	1
1:A:748:LEU:HD12	1:A:751:GLY:HA3	0.44	1.90	3	1
1:B:774:LEU:HD11	1:C:742:ARG:NE	0.44	2.28	3	1
1:C:675:ILE:HD12	1:C:679:LEU:HD12	0.44	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:660:LEU:HD23	1:C:660:LEU:N	0.44	2.28	5	1
1:B:660:LEU:N	1:B:660:LEU:HD12	0.44	2.27	7	1
1:A:748:LEU:HD13	1:A:748:LEU:C	0.44	2.32	15	1
1:A:660:LEU:CB	1:C:663:LEU:HD23	0.44	2.42	12	2
1:C:742:ARG:O	1:C:746:ILE:HD13	0.44	2.13	6	2
1:B:663:LEU:HD12	1:C:660:LEU:HD13	0.44	1.90	6	2
1:A:661:LEU:N	1:A:661:LEU:HD12	0.43	2.27	7	1
1:A:763:LEU:HB2	1:A:771:LEU:HD13	0.43	1.90	8	1
1:C:767:SER:O	1:C:768:TYR:C	0.43	2.55	13	1
1:A:768:TYR:CE1	1:A:771:LEU:HD22	0.43	2.48	3	2
1:A:669:LEU:HD23	1:A:676:THR:OG1	0.43	2.13	13	1
1:B:663:LEU:HD23	1:B:664:ASP:N	0.43	2.28	11	3
1:B:755:LEU:C	1:B:755:LEU:HD13	0.43	2.34	13	2
1:C:761:ARG:O	1:C:765:LEU:HD13	0.43	2.13	8	1
1:B:696:ARG:N	1:B:696:ARG:HD2	0.43	2.28	9	1
1:B:768:TYR:CE2	1:B:771:LEU:HD13	0.43	2.48	1	1
1:B:758:ASP:OD2	1:C:715:LEU:HD23	0.43	2.14	10	1
1:B:705:VAL:HG13	1:B:748:LEU:HD22	0.43	1.91	4	1
1:A:755:LEU:C	1:A:755:LEU:HD23	0.43	2.34	8	2
1:A:775:LEU:O	1:A:778:VAL:HG22	0.43	2.13	8	1
1:A:693:ILE:HD11	1:B:696:ARG:CG	0.43	2.43	10	1
1:A:704:LEU:HD13	1:A:707:ARG:HH22	0.43	1.73	11	1
1:A:684:ILE:HD12	1:A:684:ILE:N	0.43	2.29	4	3
1:A:762:SER:O	1:A:774:LEU:HD13	0.43	2.13	9	1
1:A:705:VAL:CG2	1:A:748:LEU:HD23	0.43	2.40	3	1
1:C:679:LEU:HD23	1:C:679:LEU:O	0.43	2.14	5	2
1:A:784:LEU:HD22	1:A:784:LEU:H	0.43	1.74	7	1
1:A:673:PHE:O	1:A:673:PHE:CG	0.43	2.71	3	1
1:C:675:ILE:HD11	1:C:678:TRP:CE3	0.43	2.48	13	3
1:B:748:LEU:C	1:B:748:LEU:HD12	0.43	2.33	9	2
1:B:663:LEU:C	1:B:663:LEU:HD23	0.43	2.34	8	1
1:A:781:ILE:HD11	1:B:746:ILE:HG21	0.43	1.90	11	1
1:C:669:LEU:HD22	1:C:669:LEU:N	0.43	2.29	2	2
1:A:660:LEU:HB2	1:C:663:LEU:HD21	0.43	1.91	3	1
1:C:746:ILE:O	1:C:749:VAL:HG23	0.43	2.14	10	1
1:A:768:TYR:CZ	1:A:771:LEU:HD22	0.43	2.49	14	1
1:B:693:ILE:HD13	1:B:693:ILE:O	0.42	2.14	5	1
1:A:748:LEU:HD23	1:B:714:PRO:HG3	0.42	1.91	10	1
1:A:705:VAL:HG13	1:A:748:LEU:HD12	0.42	1.91	13	1
1:A:777:ILE:HD11	1:B:742:ARG:NH1	0.42	2.29	1	1
1:B:760:LEU:C	1:B:760:LEU:HD13	0.42	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:774:LEU:HD11	1:C:742:ARG:NH2	0.42	2.30	13	1
1:B:693:ILE:C	1:B:693:ILE:HD12	0.42	2.35	4	1
1:C:748:LEU:C	1:C:748:LEU:HD12	0.42	2.35	4	1
1:A:768:TYR:CE1	1:A:771:LEU:HD13	0.42	2.49	11	1
1:C:684:ILE:N	1:C:684:ILE:HD12	0.42	2.28	13	1
1:B:775:LEU:HD13	1:B:775:LEU:C	0.42	2.35	14	1
1:A:747:ARG:CZ	1:A:750:ASN:CG	0.42	2.88	2	1
1:B:763:LEU:HG	1:B:774:LEU:HD22	0.42	1.90	10	1
1:B:782:VAL:HG11	1:C:749:VAL:HG11	0.42	1.91	14	2
1:C:764:SER:OG	1:C:771:LEU:HD12	0.42	2.14	5	1
1:A:755:LEU:HD21	1:B:710:GLN:NE2	0.42	2.29	7	1
1:B:706:ASN:O	1:B:710:GLN:HG2	0.42	2.15	14	2
1:A:749:VAL:HG23	1:A:750:ASN:N	0.42	2.30	11	1
1:C:705:VAL:HG13	1:C:748:LEU:HD11	0.42	1.92	12	1
1:B:689:VAL:O	1:B:692:LEU:CD1	0.42	2.67	14	3
1:C:765:LEU:O	1:C:766:PHE:C	0.42	2.59	6	2
1:A:746:ILE:O	1:A:749:VAL:CG2	0.42	2.68	8	1
1:A:712:TYR:CD1	1:C:707:ARG:CZ	0.42	3.03	9	1
1:C:763:LEU:HD21	1:C:771:LEU:HD12	0.42	1.91	12	1
1:A:713:SER:HA	1:C:708:VAL:HG21	0.42	1.91	14	1
1:A:685:PHE:O	1:A:689:VAL:HG23	0.42	2.15	15	1
1:B:715:LEU:HD23	1:B:715:LEU:O	0.41	2.15	6	1
1:B:682:ILE:N	1:B:682:ILE:HD13	0.41	2.30	10	2
1:A:697:ILE:O	1:A:697:ILE:HD13	0.41	2.15	9	1
1:C:684:ILE:O	1:C:688:ILE:HD13	0.41	2.15	2	1
1:C:705:VAL:HG13	1:C:748:LEU:HD13	0.41	1.92	2	1
1:A:747:ARG:CD	1:C:782:VAL:HA	0.41	2.45	13	1
1:A:758:ASP:HB3	1:B:710:GLN:HB2	0.41	1.92	1	2
1:C:704:LEU:HD13	1:C:704:LEU:O	0.41	2.15	1	1
1:C:775:LEU:O	1:C:778:VAL:HG12	0.41	2.15	2	1
1:B:778:VAL:HG23	1:C:746:ILE:CG1	0.41	2.45	6	1
1:B:689:VAL:O	1:B:692:LEU:HD12	0.41	2.14	9	1
1:C:768:TYR:CZ	1:C:771:LEU:HD13	0.41	2.50	15	1
1:A:693:ILE:HG22	1:C:693:ILE:HB	0.41	1.92	5	1
1:B:774:LEU:HG	1:B:777:ILE:HD11	0.41	1.92	11	1
1:A:712:TYR:CZ	1:C:707:ARG:NH1	0.41	2.89	14	1
1:A:776:LEU:HD12	1:A:776:LEU:N	0.41	2.30	15	1
1:B:669:LEU:HD22	1:B:669:LEU:N	0.41	2.30	8	1
1:B:706:ASN:O	1:B:710:GLN:HB2	0.41	2.15	8	1
1:A:678:TRP:CD1	1:A:678:TRP:C	0.41	2.94	9	1
1:B:713:SER:O	1:B:714:PRO:C	0.41	2.59	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:675:ILE:HD12	1:A:678:TRP:CE3	0.41	2.50	1	1
1:A:746:ILE:CD1	1:C:781:ILE:HD12	0.41	2.46	5	1
1:A:693:ILE:HG22	1:C:693:ILE:CB	0.41	2.46	5	1
1:C:764:SER:O	1:C:765:LEU:HB3	0.41	2.16	5	1
1:A:768:TYR:CE2	1:A:771:LEU:HD13	0.41	2.50	12	1
1:B:663:LEU:HD23	1:B:663:LEU:C	0.41	2.36	12	1
1:A:763:LEU:HB2	1:A:771:LEU:HD12	0.41	1.92	14	1
1:B:755:LEU:HD21	1:C:710:GLN:HE22	0.41	1.76	1	1
1:B:762:SER:O	1:B:774:LEU:HD22	0.41	2.16	2	1
1:A:705:VAL:HG22	1:A:748:LEU:CD2	0.41	2.41	3	1
1:C:715:LEU:HD23	1:C:715:LEU:O	0.41	2.15	4	1
1:A:713:SER:CB	1:C:708:VAL:HG23	0.41	2.46	7	1
1:B:745:SER:O	1:B:748:LEU:HD23	0.41	2.15	13	2
1:C:713:SER:O	1:C:714:PRO:C	0.41	2.59	13	1
1:C:748:LEU:HD13	1:C:748:LEU:O	0.41	2.16	1	1
1:A:684:ILE:O	1:A:688:ILE:HD13	0.41	2.16	5	1
1:C:763:LEU:HD23	1:C:763:LEU:C	0.41	2.36	10	1
1:C:684:ILE:HD12	1:C:684:ILE:N	0.41	2.31	14	1
1:B:774:LEU:HD21	1:C:742:ARG:CZ	0.40	2.47	2	1
1:A:765:LEU:C	1:A:765:LEU:HD23	0.40	2.36	3	1
1:A:693:ILE:HD11	1:B:696:ARG:NE	0.40	2.30	4	1
1:B:758:ASP:OD1	1:C:715:LEU:HD22	0.40	2.15	4	1
1:B:677:ASN:OD1	1:B:681:TYR:CZ	0.40	2.74	6	1
1:C:776:LEU:C	1:C:776:LEU:HD23	0.40	2.36	6	1
1:C:774:LEU:HD13	1:C:777:ILE:HD12	0.40	1.93	7	1
1:A:763:LEU:O	1:A:774:LEU:HD23	0.40	2.16	8	1
1:B:704:LEU:HD11	1:C:712:TYR:O	0.40	2.16	12	1
1:A:777:ILE:O	1:A:781:ILE:HD13	0.40	2.15	8	1
1:B:745:SER:O	1:B:748:LEU:HD12	0.40	2.16	5	1
1:B:708:VAL:HG11	1:B:748:LEU:HD12	0.40	1.93	1	1
1:B:679:LEU:O	1:B:682:ILE:HD12	0.40	2.16	10	1
1:C:679:LEU:O	1:C:679:LEU:HD13	0.40	2.17	12	1
1:B:775:LEU:O	1:B:778:VAL:HG22	0.40	2.17	14	1
1:B:771:LEU:C	1:B:771:LEU:HD23	0.40	2.37	1	1
1:C:705:VAL:HG13	1:C:748:LEU:CD1	0.40	2.47	2	1
1:A:675:ILE:CD1	1:A:679:LEU:HD23	0.40	2.46	4	1
1:B:660:LEU:O	1:B:661:LEU:HD22	0.40	2.16	4	1
1:C:660:LEU:HD12	1:C:660:LEU:O	0.40	2.16	9	1
1:A:663:LEU:HD23	1:A:664:ASP:N	0.40	2.32	14	1
1:A:781:ILE:HG13	1:B:746:ILE:HG21	0.40	1.92	15	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	101/129 (78%)	93±1 (92±1%)	6±1 (5±1%)	2±1 (2±1%)	9	48
1	B	103/129 (80%)	95±2 (92±2%)	5±2 (5±2%)	3±1 (3±1%)	8	42
1	C	99/129 (77%)	92±1 (93±1%)	4±1 (4±1%)	3±1 (3±1%)	7	40
All	All	4545/5805 (78%)	4207 (93%)	215 (5%)	123 (3%)	8	43

All 24 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	661	LEU	14
1	C	714	PRO	13
1	A	661	LEU	11
1	A	714	PRO	11
1	B	714	PRO	11
1	B	766	PHE	8
1	C	661	LEU	8
1	C	766	PHE	8
1	A	765	LEU	7
1	C	768	TYR	4
1	C	767	SER	4
1	C	765	LEU	4
1	A	712	TYR	3
1	B	765	LEU	3
1	B	662	GLU	3
1	B	767	SER	2
1	C	674	ASP	2
1	B	673	PHE	1
1	B	674	ASP	1
1	A	767	SER	1
1	A	768	TYR	1
1	C	673	PHE	1
1	C	769	HIS	1
1	A	674	ASP	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	97/117 (83%)	76±3 (78±3%)	21±3 (22±3%)	3	30
1	B	99/117 (85%)	77±4 (78±4%)	22±4 (22±4%)	3	30
1	C	95/117 (81%)	77±3 (81±3%)	18±3 (19±3%)	4	35
All	All	4365/5265 (83%)	3444 (79%)	921 (21%)	3	32

All 215 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	C	685	PHE	15
1	A	704	LEU	14
1	B	685	PHE	14
1	B	692	LEU	14
1	A	712	TYR	14
1	A	685	PHE	13
1	B	704	LEU	13
1	C	704	LEU	13
1	B	693	ILE	13
1	C	675	ILE	13
1	A	693	ILE	12
1	C	780	ARG	12
1	A	692	LEU	12
1	B	780	ARG	12
1	B	701	VAL	12
1	B	697	ILE	11
1	B	774	LEU	11
1	A	744	ARG	10
1	A	763	LEU	10
1	B	679	LEU	10
1	B	787	ARG	10
1	C	708	VAL	10
1	A	679	LEU	10
1	A	715	LEU	10
1	C	660	LEU	9
1	A	780	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	B	741	ASP	9
1	A	741	ASP	9
1	B	695	LEU	9
1	B	768	TYR	9
1	A	695	LEU	8
1	A	747	ARG	8
1	B	744	ARG	8
1	B	775	LEU	8
1	C	663	LEU	8
1	C	707	ARG	8
1	A	785	LEU	8
1	C	772	ARG	8
1	B	747	ARG	7
1	C	679	LEU	7
1	C	763	LEU	7
1	C	774	LEU	7
1	A	660	LEU	7
1	A	708	VAL	7
1	B	763	LEU	7
1	A	764	SER	7
1	C	662	GLU	7
1	B	765	LEU	7
1	C	678	TRP	7
1	A	699	PHE	6
1	A	771	LEU	6
1	B	766	PHE	6
1	C	748	LEU	6
1	C	768	TYR	6
1	A	664	ASP	6
1	B	660	LEU	6
1	B	708	VAL	6
1	C	674	ASP	6
1	A	665	LYS	5
1	A	698	VAL	5
1	A	743	ASP	5
1	A	746	ILE	5
1	A	748	LEU	5
1	B	713	SER	5
1	B	743	ASP	5
1	C	701	VAL	5
1	A	740	ARG	5
1	B	663	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	C	692	LEU	5
1	B	748	LEU	5
1	C	668	SER	5
1	B	662	GLU	5
1	A	710	GLN	5
1	A	683	ARG	4
1	B	769	HIS	4
1	C	710	GLN	4
1	C	739	GLU	4
1	C	766	PHE	4
1	B	760	LEU	4
1	B	772	ARG	4
1	C	760	LEU	4
1	A	662	GLU	4
1	A	663	LEU	4
1	A	774	LEU	4
1	B	665	LYS	4
1	B	739	GLU	4
1	C	665	LYS	4
1	C	744	ARG	4
1	C	746	ILE	4
1	C	764	SER	4
1	C	765	LEU	4
1	C	776	LEU	4
1	C	673	PHE	4
1	C	741	ASP	4
1	A	682	ILE	4
1	B	698	VAL	4
1	B	742	ARG	4
1	A	678	TRP	3
1	B	740	ARG	3
1	B	779	THR	3
1	C	775	LEU	3
1	A	742	ARG	3
1	C	680	TRP	3
1	B	673	PHE	3
1	B	770	ARG	3
1	C	715	LEU	3
1	B	785	LEU	3
1	A	768	TYR	3
1	A	772	ARG	3
1	B	752	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	C	693	ILE	3
1	A	675	ILE	3
1	A	767	SER	3
1	C	691	SER	3
1	C	709	ARG	3
1	C	745	SER	3
1	B	675	ILE	3
1	B	746	ILE	3
1	B	764	SER	3
1	A	702	LEU	3
1	A	765	LEU	3
1	B	678	TRP	3
1	A	776	LEU	2
1	A	777	ILE	2
1	B	778	VAL	2
1	C	697	ILE	2
1	A	674	ASP	2
1	B	674	ASP	2
1	B	710	GLN	2
1	C	661	LEU	2
1	C	740	ARG	2
1	A	779	THR	2
1	B	683	ARG	2
1	B	712	TYR	2
1	A	671	ASN	2
1	B	661	LEU	2
1	B	668	SER	2
1	B	671	ASN	2
1	B	709	ARG	2
1	C	757	TRP	2
1	A	709	ARG	2
1	A	762	SER	2
1	A	770	ARG	2
1	A	784	LEU	2
1	B	696	ARG	2
1	C	747	ARG	2
1	C	749	VAL	2
1	C	770	ARG	2
1	A	749	VAL	2
1	B	761	ARG	2
1	C	759	ASP	2
1	C	771	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	703	SER	2
1	B	664	ASP	2
1	B	682	ILE	2
1	C	767	SER	2
1	C	781	ILE	2
1	A	705	VAL	2
1	A	769	HIS	2
1	A	781	ILE	2
1	C	713	SER	2
1	C	777	ILE	2
1	A	755	LEU	2
1	A	773	ASP	2
1	A	716	SER	2
1	C	779	THR	2
1	A	669	LEU	2
1	A	775	LEU	1
1	A	668	SER	1
1	A	714	PRO	1
1	C	773	ASP	1
1	A	745	SER	1
1	C	743	ASP	1
1	B	716	SER	1
1	B	771	LEU	1
1	C	688	ILE	1
1	A	696	ARG	1
1	A	713	SER	1
1	C	669	LEU	1
1	C	671	ASN	1
1	B	788	ARG	1
1	C	783	GLU	1
1	A	676	THR	1
1	A	701	VAL	1
1	A	739	GLU	1
1	A	766	PHE	1
1	B	691	SER	1
1	B	749	VAL	1
1	B	757	TRP	1
1	A	686	ILE	1
1	A	707	ARG	1
1	A	783	GLU	1
1	B	680	TRP	1
1	B	745	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	B	776	LEU	1
1	B	777	ILE	1
1	C	742	ARG	1
1	A	697	ILE	1
1	B	762	SER	1
1	B	773	ASP	1
1	B	755	LEU	1
1	B	781	ILE	1
1	B	783	GLU	1
1	C	705	VAL	1
1	C	706	ASN	1
1	B	715	LEU	1
1	C	683	ARG	1
1	C	716	SER	1
1	A	688	ILE	1
1	B	759	ASP	1
1	A	661	LEU	1
1	A	760	LEU	1
1	B	707	ARG	1
1	C	762	SER	1
1	C	769	HIS	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 10% for the well-defined parts and 10% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *HIV1_gp41_MPER-TMD-CTLLP2_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	520
Number of shifts mapped to atoms	520
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
$^{13}\text{C}_\alpha$	120	0.00 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	55	1.27 ± 0.09	Should be applied
$^{13}\text{C}'$	113	-0.13 ± 0.14	None needed (< 0.5 ppm)
^{15}N	116	0.72 ± 0.17	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 10%, i.e. 414 atoms were assigned a chemical shift out of a possible 4292. 0 out of 88 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	379/1559 (24%)	96/623 (15%)	187/626 (30%)	96/310 (31%)
Sidechain	35/2313 (2%)	0/1341 (0%)	35/840 (4%)	0/132 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/420 (0%)	0/216 (0%)	0/180 (0%)	0/24 (0%)
Overall	414/4292 (10%)	96/2180 (4%)	222/1646 (13%)	96/466 (21%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 427 atoms were assigned a chemical shift out of a possible 4422. 0 out of 90 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	390/1599 (24%)	99/639 (15%)	192/642 (30%)	99/318 (31%)
Sidechain	37/2403 (2%)	0/1395 (0%)	37/864 (4%)	0/144 (0%)
Aromatic	0/420 (0%)	0/216 (0%)	0/180 (0%)	0/24 (0%)
Overall	427/4422 (10%)	99/2250 (4%)	229/1686 (14%)	99/486 (20%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:

