



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2020 – 11:33 am BST

PDB ID : 6V4T
Title : MPER-TMD of HIV-1 Env bound with the entry inhibitor S2C3
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Deposited on : 2019-11-30

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

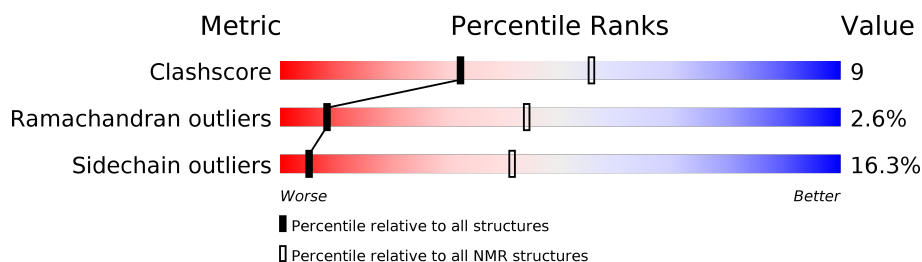
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 5%.

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	51	<div> <div style="width: 71%; background-color: green;"></div> <div style="width: 29%; background-color: yellow;"></div> </div> <div>71% 29%</div>
1	B	51	<div> <div style="width: 76%; background-color: green;"></div> <div style="width: 24%; background-color: yellow;"></div> </div> <div>76% 24%</div>
1	C	51	<div> <div style="width: 67%; background-color: green;"></div> <div style="width: 31%; background-color: yellow;"></div> <div style="width: 2%; background-color: cyan;"></div> </div> <div>67% 31% .</div>

2 Ensemble composition and analysis

This entry contains 14 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:660-A:710, B:660-B:710, C:660-C:709 (152)	1.06	1

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

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

The models can be grouped into 2 clusters and 10 single-model clusters were found.

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

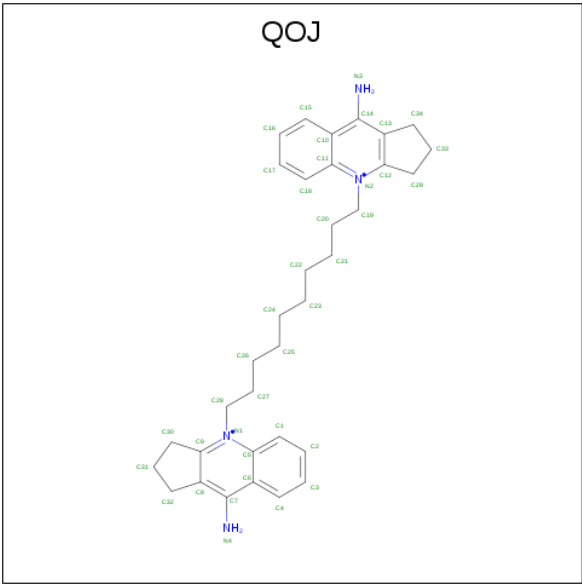
3 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2958 atoms, of which 1521 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					Trace
1	A	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	B	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	C	51	Total	C	H	N	O	0
			904	301	463	73	67	

- Molecule 2 is 4-[10-(9-azanyl-2,3-dihydro-1 {H}-cyclopenta[b]quinolin-4-yl)decyl]-2,3-dihydro-1 {H}-cyclopenta[b]quinolin-9-amine (three-letter code: QOJ) (formula: C₃₄H₄₄N₄) (labeled as "Ligand of Interest" by author).



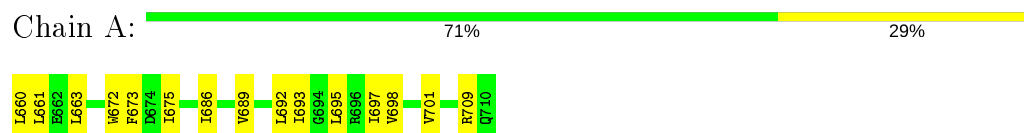
Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	N
			82	34	44	4
2	B	1	Total	C	H	N
			82	34	44	4
2	C	1	Total	C	H	N
			82	34	44	4

4 Residue-property plots [i](#)

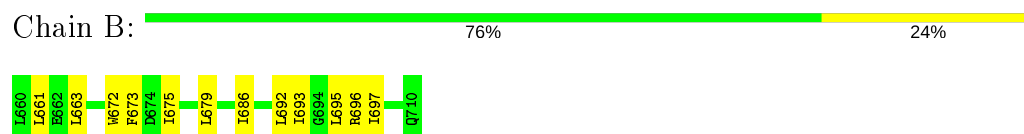
4.1 Average score per residue in the NMR ensemble

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

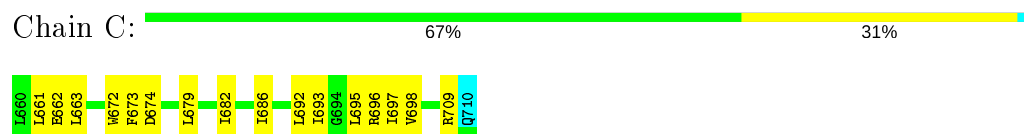
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

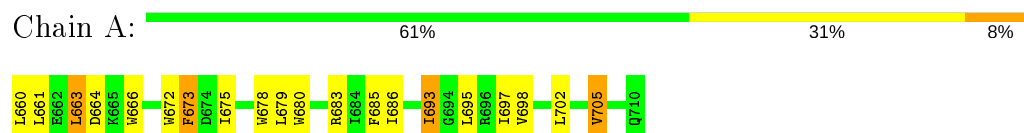


4.2 Scores per residue for each member of the ensemble

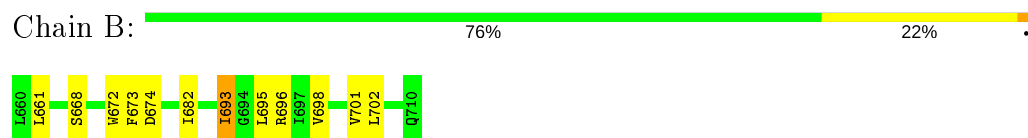
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

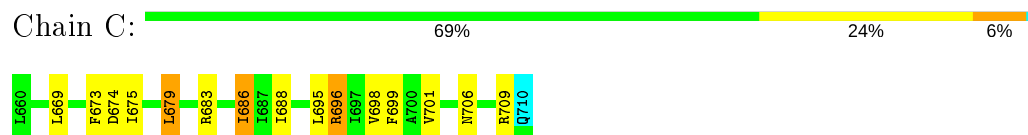
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

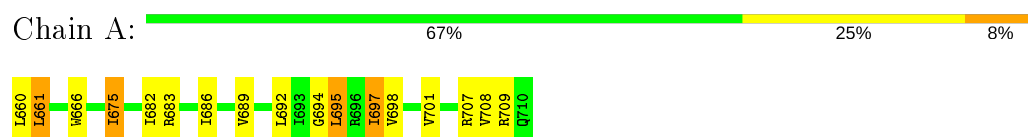


- Molecule 1: Envelope glycoprotein gp160

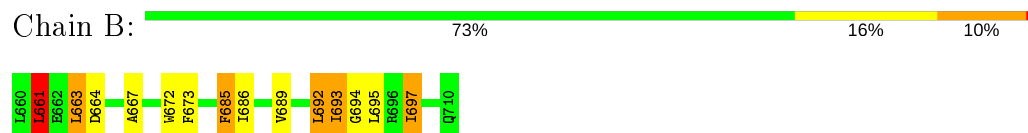


4.2.2 Score per residue for model 2

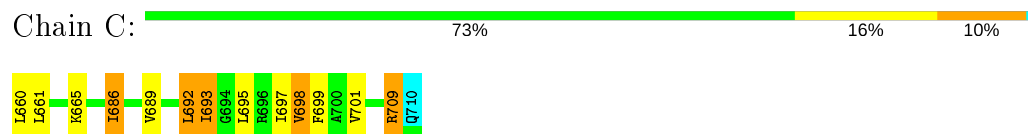
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

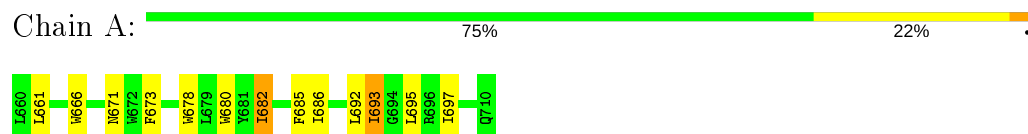


- Molecule 1: Envelope glycoprotein gp160



4.2.3 Score per residue for model 3

- Molecule 1: Envelope glycoprotein gp160



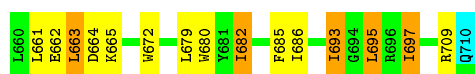
- Molecule 1: Envelope glycoprotein gp160

Chain B:  67% 29% .



- Molecule 1: Envelope glycoprotein gp160

Chain C:  69% 20% 10% .



4.2.4 Score per residue for model 4

- Molecule 1: Envelope glycoprotein gp160

Chain A:  69% 25% 6% .



- Molecule 1: Envelope glycoprotein gp160

Chain B:  69% 29% .



- Molecule 1: Envelope glycoprotein gp160

Chain C:  53% 29% 16% .



4.2.5 Score per residue for model 5

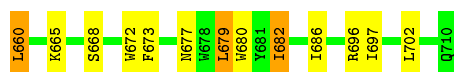
- Molecule 1: Envelope glycoprotein gp160

Chain A:  69% 25% 6% .



- Molecule 1: Envelope glycoprotein gp160

Chain B:  75% 20% 6% .



- Molecule 1: Envelope glycoprotein gp160

Chain C: 76% 16% 6%



4.2.6 Score per residue for model 6

- Molecule 1: Envelope glycoprotein gp160

Chain A: 65% 29% 6%



- Molecule 1: Envelope glycoprotein gp160

Chain B: 69% 31%



- Molecule 1: Envelope glycoprotein gp160

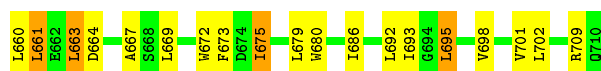
Chain C: 78% 16%



4.2.7 Score per residue for model 7

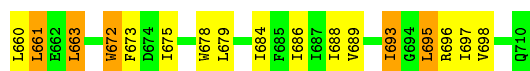
- Molecule 1: Envelope glycoprotein gp160

Chain A: 63% 29% 8%

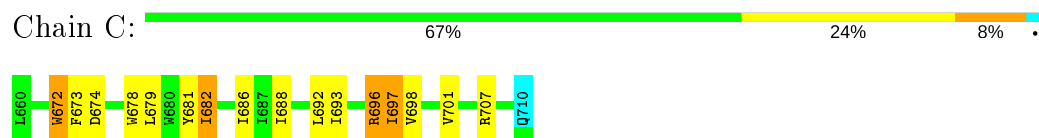


- Molecule 1: Envelope glycoprotein gp160

Chain B: 67% 24% 10%

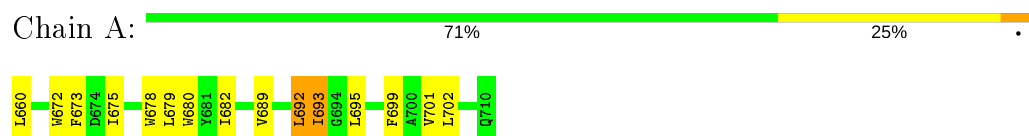


- Molecule 1: Envelope glycoprotein gp160

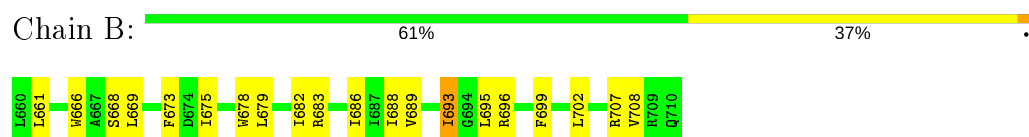


4.2.8 Score per residue for model 8

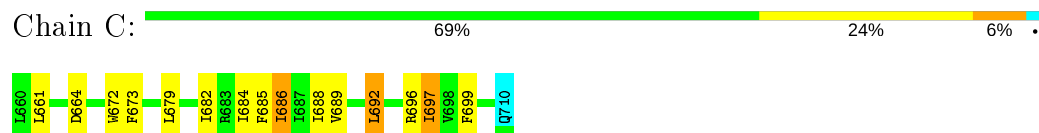
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

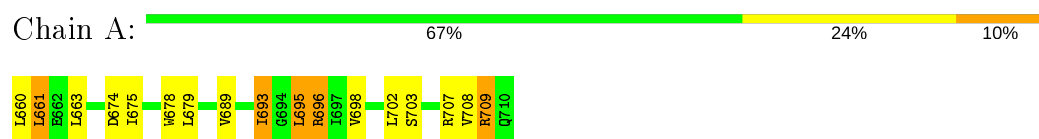


- Molecule 1: Envelope glycoprotein gp160

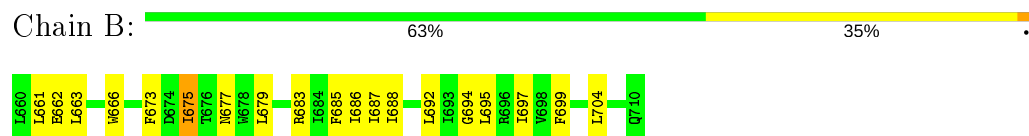


4.2.9 Score per residue for model 9

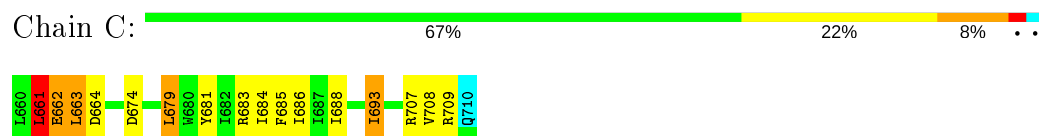
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

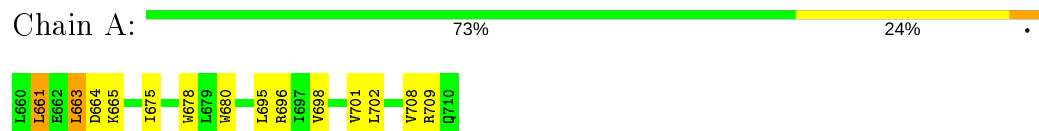


- Molecule 1: Envelope glycoprotein gp160

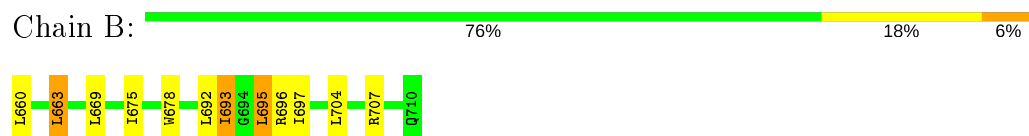


4.2.10 Score per residue for model 10

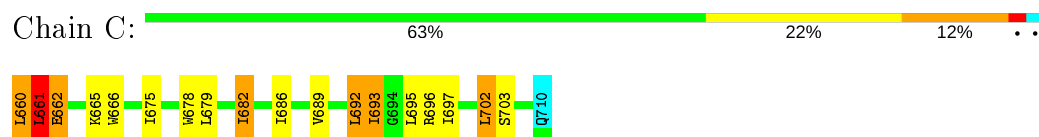
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

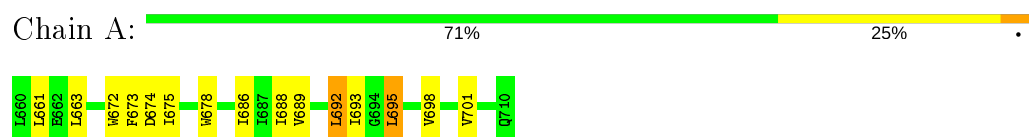


- Molecule 1: Envelope glycoprotein gp160

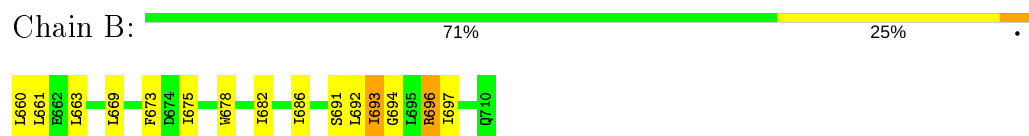


4.2.11 Score per residue for model 11

- Molecule 1: Envelope glycoprotein gp160

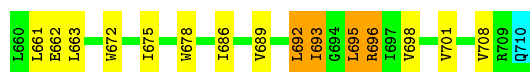


- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160





4.2.12 Score per residue for model 12

- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

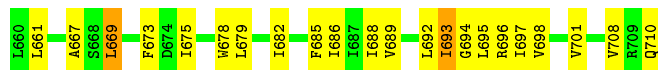


4.2.13 Score per residue for model 13

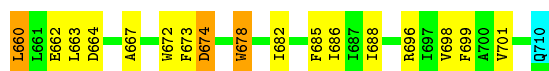
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160




4.2.14 Score per residue for model 14

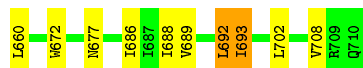
- Molecule 1: Envelope glycoprotein gp160

Chain A:  67% 25% 8%



- Molecule 1: Envelope glycoprotein gp160

Chain B:  80% 16% .



- Molecule 1: Envelope glycoprotein gp160

Chain C:  73% 22% . .



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 14 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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	96
Number of shifts mapped to atoms	96
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	5%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	441	463	460	10±3
1	B	441	463	460	10±3
1	C	431	455	452	12±3
2	A	38	44	0	0±1
2	C	38	44	0	0±1
All	All	19978	21182	19208	370

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:692:LEU:HD13	1:C:693:ILE:N	0.79	1.92	4	4
1:B:686:ILE:HG21	1:C:686:ILE:HD11	0.75	1.58	5	2
1:B:686:ILE:HG21	1:C:686:ILE:HD12	0.75	1.56	11	5
1:A:661:LEU:HD13	1:C:666:TRP:NE1	0.72	2.00	10	1
1:A:698:VAL:O	1:A:701:VAL:HG22	0.71	1.84	10	2
1:A:663:LEU:HD13	1:A:664:ASP:N	0.71	2.00	1	3
1:B:669:LEU:HD21	1:B:675:ILE:HG23	0.70	1.63	6	1
1:A:695:LEU:O	1:A:698:VAL:HG12	0.69	1.87	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:682:ILE:HD12	1:C:683:ARG:N	0.68	2.03	12	1
1:A:702:LEU:O	1:A:705:VAL:HG12	0.68	1.89	4	2
1:A:661:LEU:HD11	1:A:666:TRP:CZ2	0.68	2.24	1	1
1:C:666:TRP:O	1:C:669:LEU:HD12	0.68	1.88	4	1
1:A:695:LEU:O	1:A:698:VAL:HG22	0.68	1.89	2	6
1:B:678:TRP:O	1:B:682:ILE:HG23	0.68	1.89	11	3
1:C:695:LEU:O	1:C:695:LEU:HD22	0.67	1.90	3	2
1:C:693:ILE:HD13	1:C:693:ILE:O	0.67	1.89	5	5
1:A:693:ILE:HD13	1:A:693:ILE:O	0.67	1.89	13	3
1:C:663:LEU:HD22	1:C:663:LEU:O	0.67	1.90	9	1
1:A:689:VAL:O	1:A:692:LEU:HD11	0.66	1.91	8	3
1:C:698:VAL:O	1:C:701:VAL:HG12	0.66	1.91	7	4
1:C:689:VAL:O	1:C:692:LEU:HD12	0.66	1.90	2	4
1:C:663:LEU:HD13	1:C:664:ASP:N	0.66	2.06	9	2
1:C:669:LEU:HD13	1:C:670:TRP:N	0.65	2.07	4	1
1:B:693:ILE:HD13	1:B:693:ILE:O	0.64	1.92	2	3
1:A:693:ILE:O	1:A:693:ILE:HD13	0.64	1.91	8	4
1:B:695:LEU:HD22	1:B:695:LEU:C	0.64	2.12	3	2
1:A:663:LEU:HD13	1:A:664:ASP:H	0.63	1.53	10	1
1:A:686:ILE:HG21	1:B:686:ILE:HD11	0.63	1.68	7	1
1:C:682:ILE:HD13	1:C:682:ILE:O	0.63	1.93	7	1
1:A:686:ILE:CG2	1:B:686:ILE:HD11	0.63	2.23	7	1
1:C:697:ILE:HD13	1:C:697:ILE:O	0.63	1.94	3	2
1:B:669:LEU:HD11	1:B:675:ILE:HG23	0.63	1.70	8	2
1:C:693:ILE:O	1:C:693:ILE:HD13	0.63	1.92	11	3
1:B:666:TRP:CG	1:C:661:LEU:HD12	0.62	2.30	9	1
1:C:697:ILE:O	1:C:697:ILE:HD13	0.62	1.95	14	3
1:B:697:ILE:HD13	1:C:696:ARG:NH1	0.61	2.10	10	1
1:A:660:LEU:CD1	1:C:667:ALA:HB2	0.61	2.26	13	1
1:C:681:TYR:HB2	1:C:684:ILE:HD12	0.61	1.73	9	1
1:C:669:LEU:HD22	1:C:669:LEU:O	0.61	1.95	4	1
1:B:669:LEU:HD21	1:B:675:ILE:CG2	0.60	2.26	6	1
1:C:698:VAL:O	1:C:701:VAL:HG22	0.60	1.96	2	2
1:A:686:ILE:HD11	1:C:686:ILE:CG2	0.60	2.26	1	2
1:C:692:LEU:HD13	1:C:693:ILE:H	0.60	1.56	2	4
1:B:694:GLY:O	1:B:697:ILE:HG22	0.60	1.97	4	6
1:A:686:ILE:CD1	1:C:686:ILE:HG21	0.59	2.27	14	1
1:B:697:ILE:HD13	1:B:697:ILE:O	0.59	1.97	2	1
1:C:663:LEU:HD22	1:C:664:ASP:N	0.59	2.13	3	1
1:A:695:LEU:C	1:A:695:LEU:HD22	0.59	2.18	7	1
1:A:661:LEU:HD11	2:A:801:QOJ:C9	0.59	2.27	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:697:ILE:O	1:A:697:ILE:HD13	0.59	1.97	2	1
1:B:693:ILE:HD11	1:C:696:ARG:HG3	0.59	1.75	14	2
1:A:686:ILE:HG23	1:C:686:ILE:HG12	0.59	1.75	3	1
1:B:669:LEU:HD22	1:B:675:ILE:HG21	0.59	1.74	11	1
1:A:698:VAL:O	1:A:701:VAL:HG12	0.59	1.98	5	5
1:B:685:PHE:HA	1:B:688:ILE:HD12	0.58	1.74	13	1
1:C:695:LEU:O	1:C:698:VAL:HG22	0.58	1.97	12	3
1:A:666:TRP:CD1	1:B:661:LEU:HD21	0.58	2.32	1	1
1:B:693:ILE:HD12	1:B:693:ILE:O	0.58	1.98	10	2
1:A:663:LEU:O	1:A:663:LEU:HD22	0.58	1.98	7	1
1:A:667:ALA:HB2	1:B:660:LEU:CD1	0.58	2.29	7	1
1:B:693:ILE:O	1:B:693:ILE:HD12	0.58	1.99	13	2
1:A:694:GLY:O	1:A:697:ILE:HG22	0.57	1.98	2	2
1:A:697:ILE:HD13	1:A:697:ILE:O	0.57	1.98	6	1
1:A:695:LEU:O	1:A:695:LEU:HD23	0.57	2.00	3	3
1:A:661:LEU:O	1:C:663:LEU:HD23	0.56	2.00	9	1
1:B:697:ILE:HD11	1:C:696:ARG:HD3	0.56	1.77	5	1
1:B:695:LEU:O	1:B:698:VAL:HG22	0.56	2.00	3	2
1:B:689:VAL:O	1:B:692:LEU:HD11	0.56	2.01	2	2
1:A:672:TRP:O	1:A:674:ASP:N	0.56	2.38	11	1
1:C:695:LEU:O	1:C:695:LEU:HD23	0.55	2.01	14	3
1:A:678:TRP:CD1	1:A:682:ILE:HG21	0.55	2.37	8	1
1:A:696:ARG:HG3	1:C:693:ILE:HD11	0.55	1.78	6	1
1:A:663:LEU:C	1:A:663:LEU:HD22	0.55	2.22	10	1
1:A:666:TRP:CD1	1:B:661:LEU:HD13	0.55	2.37	3	1
1:C:663:LEU:C	1:C:663:LEU:HD22	0.55	2.21	5	1
1:B:698:VAL:O	1:B:701:VAL:HG22	0.54	2.02	1	4
1:B:693:ILE:HG21	1:C:692:LEU:HD23	0.54	1.77	7	1
1:A:660:LEU:CG	1:C:663:LEU:HD23	0.54	2.33	5	1
1:A:682:ILE:HD12	1:A:683:ARG:N	0.54	2.18	2	3
1:A:697:ILE:HD11	1:B:699:PHE:CB	0.54	2.33	12	1
1:C:681:TYR:CB	1:C:684:ILE:HD12	0.53	2.33	9	1
1:A:661:LEU:HD23	1:A:666:TRP:CZ2	0.53	2.38	5	1
1:B:695:LEU:HD22	1:B:696:ARG:N	0.53	2.18	10	1
1:B:693:ILE:HD11	1:C:696:ARG:HD3	0.53	1.78	11	1
1:B:663:LEU:HD12	1:B:664:ASP:N	0.53	2.19	4	1
1:A:669:LEU:HD21	1:A:675:ILE:HG22	0.53	1.81	14	1
1:B:663:LEU:HD22	1:B:663:LEU:C	0.53	2.23	10	2
1:B:679:LEU:HD22	1:B:682:ILE:HG13	0.53	1.81	3	1
1:A:697:ILE:HD11	1:B:699:PHE:HB3	0.52	1.81	12	1
1:C:689:VAL:O	1:C:692:LEU:HD11	0.52	2.05	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.52	1.82	13	1
1:A:675:ILE:HD13	1:A:675:ILE:O	0.51	2.06	6	4
1:B:672:TRP:CZ3	1:B:675:ILE:HG22	0.51	2.40	7	1
1:B:669:LEU:CD1	1:B:675:ILE:HG23	0.51	2.35	13	2
1:B:663:LEU:C	1:B:663:LEU:HD22	0.51	2.25	7	1
1:B:663:LEU:HD23	1:B:663:LEU:O	0.51	2.05	9	1
1:A:675:ILE:HD12	1:A:679:LEU:CD1	0.51	2.36	6	1
1:A:661:LEU:HD23	1:A:666:TRP:CE2	0.51	2.41	5	1
1:A:663:LEU:HD22	1:A:663:LEU:C	0.51	2.26	12	2
1:A:678:TRP:O	1:A:682:ILE:HG23	0.51	2.06	13	1
1:C:690:GLY:O	1:C:693:ILE:HG22	0.50	2.06	6	1
1:C:663:LEU:HD22	1:C:663:LEU:C	0.50	2.26	3	2
1:A:686:ILE:HD11	1:C:686:ILE:HG23	0.50	1.83	1	2
1:B:693:ILE:HD11	1:C:696:ARG:CD	0.50	2.37	11	1
1:A:675:ILE:O	1:A:675:ILE:HD13	0.50	2.06	2	1
1:C:682:ILE:O	1:C:686:ILE:HD13	0.50	2.06	13	1
1:C:661:LEU:HD11	2:C:801:QOJ:C7	0.50	2.36	9	1
1:A:695:LEU:HD23	1:A:695:LEU:O	0.50	2.07	1	1
1:A:686:ILE:HD11	1:C:686:ILE:HG21	0.49	1.82	7	1
1:C:663:LEU:HD13	1:C:664:ASP:H	0.49	1.66	5	1
1:A:696:ARG:HG2	1:C:693:ILE:HD11	0.49	1.85	9	1
1:C:702:LEU:H	1:C:702:LEU:HD13	0.49	1.66	10	1
1:C:702:LEU:HD22	1:C:703:SER:N	0.49	2.22	10	1
1:A:686:ILE:HD12	1:C:686:ILE:HG21	0.49	1.84	14	1
1:A:692:LEU:HD23	1:C:693:ILE:HD11	0.49	1.84	7	1
1:A:685:PHE:O	1:A:689:VAL:HG23	0.49	2.08	14	1
1:C:679:LEU:O	1:C:679:LEU:HD13	0.49	2.06	9	2
1:B:667:ALA:HB2	1:C:660:LEU:HG	0.49	1.83	13	1
1:C:682:ILE:HD13	1:C:682:ILE:C	0.49	2.28	3	2
1:C:704:LEU:O	1:C:704:LEU:HD13	0.48	2.08	4	1
1:A:686:ILE:HG13	1:B:686:ILE:HD12	0.48	1.84	2	2
1:A:689:VAL:HG13	1:C:693:ILE:HG21	0.48	1.84	6	1
1:B:697:ILE:HD11	1:C:696:ARG:NH2	0.48	2.23	7	1
1:B:686:ILE:HG21	1:C:686:ILE:CD1	0.48	2.38	14	3
1:A:660:LEU:HG	1:C:663:LEU:HD23	0.48	1.84	5	1
1:B:675:ILE:HD12	1:B:678:TRP:CE3	0.48	2.43	7	3
1:C:685:PHE:HA	1:C:688:ILE:HD12	0.48	1.84	13	2
1:B:667:ALA:HB2	1:C:660:LEU:HD23	0.48	1.84	2	1
1:A:675:ILE:HD12	1:A:679:LEU:HD12	0.48	1.85	6	1
1:A:696:ARG:NH2	1:C:697:ILE:HD13	0.47	2.24	6	1
1:A:663:LEU:HD21	1:B:660:LEU:CD2	0.47	2.39	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:682:ILE:O	1:B:686:ILE:HD13	0.47	2.09	5	1
1:A:669:LEU:HD22	1:A:669:LEU:N	0.47	2.24	4	1
1:C:669:LEU:HD13	1:C:669:LEU:C	0.47	2.28	4	1
1:C:695:LEU:C	1:C:695:LEU:HD13	0.47	2.30	1	2
1:C:684:ILE:O	1:C:688:ILE:HD12	0.47	2.10	8	1
1:A:693:ILE:HD11	1:B:696:ARG:CG	0.47	2.39	6	1
1:C:693:ILE:HD12	1:C:693:ILE:O	0.47	2.10	9	1
1:B:660:LEU:O	1:B:661:LEU:HD22	0.47	2.09	7	1
1:B:661:LEU:HD23	1:B:661:LEU:N	0.47	2.23	1	1
1:A:675:ILE:HD11	1:A:678:TRP:CE3	0.47	2.44	8	4
1:A:689:VAL:O	1:A:689:VAL:HG12	0.47	2.10	8	3
1:A:669:LEU:HD12	1:A:669:LEU:C	0.47	2.31	6	1
1:A:708:VAL:HG12	1:A:708:VAL:O	0.47	2.10	2	2
1:A:661:LEU:HD11	2:A:801:QOJ:C30	0.46	2.39	14	1
1:B:708:VAL:O	1:B:708:VAL:HG12	0.46	2.10	8	3
1:C:708:VAL:O	1:C:708:VAL:HG12	0.46	2.11	4	3
1:A:686:ILE:CG1	1:C:686:ILE:HG21	0.46	2.40	11	1
1:A:682:ILE:HD13	1:A:682:ILE:O	0.46	2.11	3	1
1:B:688:ILE:N	1:B:688:ILE:HD12	0.46	2.26	4	3
1:A:683:ARG:NH2	1:B:679:LEU:HD22	0.46	2.26	5	1
1:A:708:VAL:O	1:A:708:VAL:HG12	0.46	2.11	12	3
1:A:660:LEU:HD22	1:A:660:LEU:N	0.46	2.26	9	1
1:A:688:ILE:HD12	1:A:688:ILE:H	0.45	1.71	11	1
1:C:675:ILE:HG23	1:C:679:LEU:HD23	0.45	1.88	1	1
1:A:663:LEU:HD13	1:A:663:LEU:C	0.45	2.32	7	1
1:B:688:ILE:H	1:B:688:ILE:HD12	0.45	1.71	9	1
1:A:669:LEU:CD2	1:A:675:ILE:HG22	0.45	2.42	14	1
1:B:693:ILE:HD13	1:B:693:ILE:C	0.45	2.31	2	1
1:A:696:ARG:NE	1:C:697:ILE:HD13	0.45	2.27	10	1
1:C:692:LEU:HD12	1:C:693:ILE:H	0.45	1.70	12	1
1:B:695:LEU:O	1:B:695:LEU:HD22	0.45	2.12	3	1
1:B:688:ILE:HD12	1:B:688:ILE:N	0.45	2.26	8	1
1:B:704:LEU:HD12	1:B:704:LEU:N	0.45	2.26	10	1
1:A:667:ALA:HB2	1:B:660:LEU:HD13	0.45	1.88	7	1
1:A:686:ILE:CG2	1:B:686:ILE:HD12	0.44	2.42	14	1
1:A:660:LEU:O	1:A:661:LEU:O	0.44	2.36	7	1
1:B:697:ILE:HD11	1:C:696:ARG:CZ	0.44	2.42	7	1
1:C:688:ILE:H	1:C:688:ILE:HD12	0.44	1.72	7	2
1:A:660:LEU:HD23	1:A:660:LEU:N	0.44	2.27	8	1
1:A:663:LEU:HD23	1:A:663:LEU:C	0.44	2.32	6	1
1:C:661:LEU:HD23	1:C:665:LYS:CG	0.44	2.43	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:707:ARG:CZ	1:C:707:ARG:CZ	0.44	2.96	14	1
1:B:675:ILE:O	1:B:675:ILE:HD13	0.44	2.13	9	1
1:C:679:LEU:HD12	1:C:679:LEU:N	0.44	2.27	5	1
1:C:697:ILE:HD12	1:C:698:VAL:N	0.44	2.27	2	1
1:B:708:VAL:HG22	1:B:708:VAL:O	0.44	2.12	3	1
1:C:693:ILE:C	1:C:693:ILE:HD13	0.44	2.33	4	2
1:B:663:LEU:HD13	1:B:664:ASP:N	0.44	2.28	2	1
1:C:660:LEU:N	1:C:660:LEU:HD23	0.44	2.28	10	1
1:C:663:LEU:C	1:C:663:LEU:HD13	0.44	2.33	9	1
1:C:693:ILE:HD12	1:C:697:ILE:HD11	0.43	1.90	10	1
1:C:672:TRP:CZ3	1:C:675:ILE:HG22	0.43	2.48	4	1
1:A:697:ILE:HD12	1:A:698:VAL:N	0.43	2.28	1	1
1:C:669:LEU:HD11	1:C:675:ILE:HG22	0.43	1.90	1	1
1:C:669:LEU:HD11	2:C:801:QOJ:C19	0.43	2.43	6	1
1:B:708:VAL:O	1:B:708:VAL:HG22	0.43	2.12	4	1
1:B:686:ILE:HG21	1:C:686:ILE:HG13	0.43	1.91	8	1
1:B:684:ILE:HD12	1:B:684:ILE:N	0.43	2.28	7	1
1:A:669:LEU:HD11	1:A:675:ILE:HG22	0.43	1.91	7	1
1:B:689:VAL:HG12	1:B:689:VAL:O	0.43	2.13	14	4
1:A:661:LEU:HD12	2:A:801:QOJ:C31	0.43	2.44	10	1
1:C:675:ILE:HD12	1:C:678:TRP:CE3	0.43	2.48	11	1
1:B:685:PHE:O	1:B:689:VAL:HG23	0.43	2.13	2	1
1:B:693:ILE:HD11	1:C:696:ARG:HG2	0.43	1.90	1	1
1:C:661:LEU:HD11	2:C:801:QOJ:C8	0.43	2.44	9	1
1:B:695:LEU:CD2	1:B:695:LEU:C	0.43	2.86	3	1
1:A:669:LEU:HD11	1:A:676:THR:OG1	0.43	2.14	14	1
1:C:672:TRP:O	1:C:674:ASP:N	0.43	2.52	14	4
1:B:684:ILE:N	1:B:684:ILE:HD12	0.43	2.29	6	1
1:B:667:ALA:HB2	1:C:660:LEU:CD2	0.42	2.44	12	1
1:B:672:TRP:O	1:B:674:ASP:N	0.42	2.52	1	2
1:A:689:VAL:HG12	1:A:689:VAL:O	0.42	2.14	9	2
1:C:663:LEU:HD23	1:C:663:LEU:C	0.42	2.35	11	1
1:C:678:TRP:C	1:C:678:TRP:CD1	0.42	2.92	13	1
1:A:693:ILE:HD11	1:B:696:ARG:HG2	0.42	1.89	11	1
1:C:695:LEU:O	1:C:698:VAL:HG23	0.42	2.15	2	1
1:A:682:ILE:CD1	1:A:686:ILE:HD11	0.42	2.44	3	1
1:B:686:ILE:CG2	1:C:686:ILE:HD11	0.42	2.44	3	1
1:A:693:ILE:HD12	1:B:696:ARG:HG3	0.42	1.90	1	1
1:C:695:LEU:HD23	1:C:695:LEU:C	0.42	2.35	10	1
1:B:692:LEU:HD12	1:B:693:ILE:H	0.42	1.75	14	1
1:A:675:ILE:HD12	1:A:678:TRP:CE3	0.42	2.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:678:TRP:O	1:C:682:ILE:HG23	0.42	2.14	10	2
1:B:688:ILE:HD12	1:B:688:ILE:H	0.42	1.73	7	1
1:B:702:LEU:HD23	1:B:702:LEU:C	0.42	2.34	1	1
1:A:686:ILE:HG21	1:B:686:ILE:CD1	0.41	2.45	14	1
1:A:704:LEU:O	1:A:704:LEU:HD23	0.41	2.15	12	1
1:A:661:LEU:O	1:C:663:LEU:HD12	0.41	2.15	11	1
1:B:686:ILE:N	1:B:686:ILE:HD12	0.41	2.30	7	1
1:C:692:LEU:HD22	1:C:692:LEU:C	0.41	2.34	2	1
1:C:660:LEU:O	1:C:661:LEU:HD12	0.41	2.15	10	1
1:C:678:TRP:O	1:C:682:ILE:HG22	0.41	2.15	7	1
1:B:686:ILE:HG21	1:C:686:ILE:CG1	0.41	2.45	13	1
1:B:660:LEU:N	1:B:660:LEU:HD23	0.41	2.31	5	1
1:B:687:ILE:HD12	1:B:687:ILE:H	0.41	1.76	9	1
1:A:696:ARG:HD3	1:C:693:ILE:HD11	0.41	1.90	9	1
1:A:669:LEU:HD22	1:A:676:THR:OG1	0.41	2.15	5	1
1:A:663:LEU:O	1:A:663:LEU:HD23	0.41	2.15	9	1
1:B:661:LEU:HD22	1:B:666:TRP:CZ2	0.41	2.50	8	1
1:B:678:TRP:CZ3	1:B:679:LEU:HD21	0.41	2.51	12	1
1:B:689:VAL:O	1:B:689:VAL:HG12	0.41	2.16	7	1
1:A:688:ILE:HD12	1:A:688:ILE:N	0.41	2.30	11	1
1:A:661:LEU:N	1:A:661:LEU:HD12	0.41	2.30	2	1
1:C:661:LEU:HD12	1:C:661:LEU:O	0.41	2.15	8	1
1:A:669:LEU:HD13	1:A:669:LEU:O	0.41	2.15	14	1
1:C:692:LEU:HD12	1:C:693:ILE:N	0.41	2.31	12	1
1:A:666:TRP:NE1	1:B:661:LEU:HD22	0.41	2.30	2	1
1:C:688:ILE:N	1:C:688:ILE:HD12	0.41	2.31	7	1
1:B:666:TRP:CD1	1:C:661:LEU:HD12	0.41	2.52	4	1
1:A:666:TRP:HE1	1:B:661:LEU:HD22	0.41	1.76	2	1
1:A:678:TRP:O	1:A:682:ILE:HG22	0.40	2.16	3	1
1:B:663:LEU:HD13	1:B:664:ASP:H	0.40	1.76	2	1
1:B:667:ALA:HB2	1:C:660:LEU:HD22	0.40	1.92	12	1
1:B:663:LEU:HD23	1:B:663:LEU:C	0.40	2.36	9	1
1:C:675:ILE:HG13	1:C:679:LEU:HD23	0.40	1.93	10	1
1:B:666:TRP:CD1	1:C:661:LEU:HD21	0.40	2.52	8	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	49/51 (96%)	45±1 (91±3%)	3±1 (6±2%)	1±1 (3±1%)	8	44
1	B	49/51 (96%)	46±1 (94±3%)	2±1 (4±2%)	1±1 (2±2%)	11	52
1	C	49/51 (96%)	46±1 (93±3%)	2±1 (3±2%)	2±1 (3±2%)	7	39
All	All	2058/2142 (96%)	1913 (93%)	92 (4%)	53 (3%)	8	44

All 13 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	673	PHE	9
1	A	673	PHE	8
1	C	673	PHE	7
1	C	709	ARG	5
1	A	661	LEU	5
1	B	661	LEU	4
1	C	681	TYR	3
1	C	661	LEU	3
1	C	662	GLU	3
1	A	662	GLU	2
1	A	709	ARG	2
1	B	662	GLU	1
1	A	681	TYR	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	47/47 (100%)	39±2 (84±5%)	8±2 (16±5%)	5	42
1	B	47/47 (100%)	39±2 (84±3%)	8±2 (16±3%)	5	42
1	C	46/47 (98%)	38±2 (83±4%)	8±2 (17±4%)	5	41
All	All	1960/1974 (99%)	1641 (84%)	319 (16%)	5	41

All 94 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	B	695	LEU	10
1	B	693	ILE	9
1	C	693	ILE	9
1	A	693	ILE	8
1	A	695	LEU	8
1	C	679	LEU	8
1	A	692	LEU	8
1	B	692	LEU	7
1	B	696	ARG	7
1	A	672	TRP	7
1	A	709	ARG	7
1	C	692	LEU	6
1	C	661	LEU	6
1	A	680	TRP	6
1	B	679	LEU	6
1	C	699	PHE	6
1	B	707	ARG	5
1	C	695	LEU	5
1	A	675	ILE	5
1	A	702	LEU	5
1	B	663	LEU	5
1	C	696	ARG	5
1	A	685	PHE	5
1	C	697	ILE	5
1	C	662	GLU	5
1	A	663	LEU	5
1	B	672	TRP	5
1	A	660	LEU	5
1	A	679	LEU	5
1	C	686	ILE	4
1	B	660	LEU	4
1	B	661	LEU	4
1	C	663	LEU	4
1	B	683	ARG	4
1	A	707	ARG	4
1	C	672	TRP	4
1	C	682	ILE	4
1	C	674	ASP	4
1	B	677	ASN	4
1	B	702	LEU	3
1	B	673	PHE	3
1	C	685	PHE	3
1	B	669	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	665	LYS	3
1	B	699	PHE	3
1	B	668	SER	3
1	C	683	ARG	3
1	B	685	PHE	3
1	C	709	ARG	3
1	C	664	ASP	3
1	C	660	LEU	3
1	A	697	ILE	3
1	A	662	GLU	2
1	A	683	ARG	2
1	B	664	ASP	2
1	A	682	ILE	2
1	C	707	ARG	2
1	A	669	LEU	2
1	C	665	LYS	2
1	A	671	ASN	2
1	A	696	ARG	2
1	A	664	ASP	2
1	B	682	ILE	2
1	C	673	PHE	2
1	B	675	ILE	2
1	B	691	SER	2
1	C	680	TRP	2
1	A	686	ILE	1
1	A	661	LEU	1
1	C	704	LEU	1
1	A	674	ASP	1
1	B	704	LEU	1
1	A	699	PHE	1
1	A	701	VAL	1
1	B	662	GLU	1
1	B	710	GLN	1
1	C	684	ILE	1
1	C	691	SER	1
1	B	706	ASN	1
1	C	669	LEU	1
1	A	676	THR	1
1	C	702	LEU	1
1	A	673	PHE	1
1	B	697	ILE	1
1	B	680	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	C	698	VAL	1
1	A	703	SER	1
1	A	665	LYS	1
1	C	675	ILE	1
1	B	674	ASP	1
1	A	681	TYR	1
1	A	705	VAL	1
1	C	678	TRP	1
1	C	706	ASN	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 carbohydrates in this entry.

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6.6 Other polymers [i](#)

There are no such molecules in this entry.

6.7 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 5% for the well-defined parts and 5% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *BMRB.txt*

7.1.1 Bookkeeping

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

Total number of shifts	96
Number of shifts mapped to atoms	96
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
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	48	1.53 ± 0.64	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 5%, i.e. 96 atoms were assigned a chemical shift out of a possible 2109. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	96/760 (13%)	48/304 (16%)	0/304 (0%)	48/152 (32%)
Sidechain	0/1064 (0%)	0/612 (0%)	0/402 (0%)	0/50 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/285 (0%)	0/147 (0%)	0/123 (0%)	0/15 (0%)
Overall	96/2109 (5%)	48/1063 (5%)	0/829 (0%)	48/217 (22%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 96 atoms were assigned a chemical shift out of a possible 2124. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	96/765 (13%)	48/306 (16%)	0/306 (0%)	48/153 (31%)
Sidechain	0/1074 (0%)	0/618 (0%)	0/405 (0%)	0/51 (0%)
Aromatic	0/285 (0%)	0/147 (0%)	0/123 (0%)	0/15 (0%)
Overall	96/2124 (5%)	48/1071 (4%)	0/834 (0%)	48/219 (22%)

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:

