Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 11:44 PM EDT

PDB ID	:	1HFN
BMRB ID	:	4914
Title	:	NMR solution structures of vMIP-II 1-71 from Kaposi's sarcoma-associated herpesvirus.
Authors	:	Crump, M.P.; Elisseeva, E.; Gong, J.-H.; Clark-Lewis, I.; Sykes, B.D.
Deposited on	:	2000-12-07

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

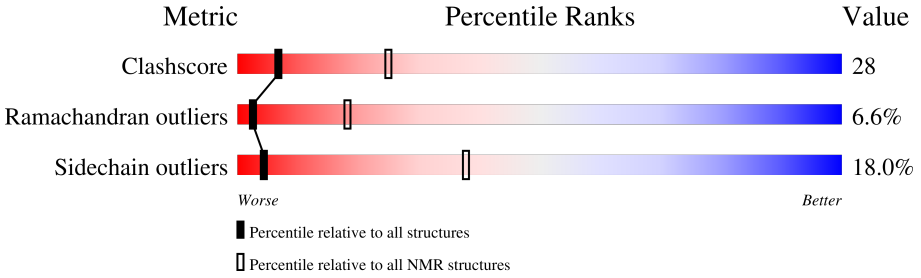
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	71	37% 41% • • 17%

2 Ensemble composition and analysis (i)

This entry contains 38 models. Model 10 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:11-A:69 (59)	0.56	10

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 5 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 5, 7, 8, 10, 13, 14, 16, 17, 19, 20, 21, 23, 24, 25, 26, 28, 31, 32, 33, 34, 35
2	1, 9, 12, 29
3	2, 4, 37, 38
4	11, 36
5	6, 18
Single-model clusters	15; 22; 27; 30

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1165 atoms, of which 595 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	71	1165	365	595	105	95	5	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 37% 41% • • 17%

L1 G2 A3 S4 W5 H6 R7 P8 D9 K10 C11 C12 Y15 Q16 L20 P21 Q22 V23 L24 L25 S26 S27 W28 Y29 S32 Q33 L34 V40 I41 F42 L43 T44 Q49 V50 C51 A52 D53 K54 S55 K56 V59 L62 M63 L66 P67 V68 T69 A70 R71

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: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 32% 42% 7% • 17%

L1 G2 A3 S4 W5 H6 R7 P8 D9 K10 C11 Y15 Q16 P19 L20 P21 Q22 V23 L24 L25 S26 S27 W28 Y29 P30 T31 S32 Q33 L34 V40 I41 F42 L43 T44 Q49 A52 D53 K54 S55 K56 V59 L62 M63 L66 P67 V68 T69 A70 R71

4.2.2 Score per residue for model 2

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

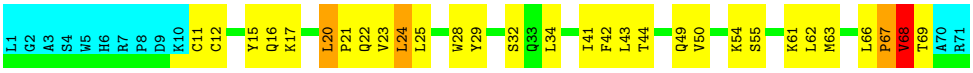
Chain A: 42% 34% 6% • 17%

L1 G2 A3 S4 W5 H6 R7 P8 D9 K10 L13 G14 Y15 Q16 L20 P21 Q22 V23 L24 L25 S26 S27 W28 Y29 L34 V40 I41 F42 L43 T44 Q49 V50 D53 K54 S55 K56 D57 W58 V59 L62 M63 P67 V68 T69 A70 R71

4.2.3 Score per residue for model 3

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

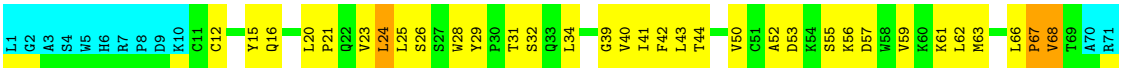
Chain A: 41% 37% • • 17%



4.2.4 Score per residue for model 4

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 37% 42% • 17%



4.2.5 Score per residue for model 5

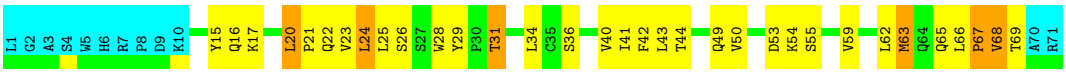
• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 45% 31% 7% 17%

4.2.6 Score per residue for model 6

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

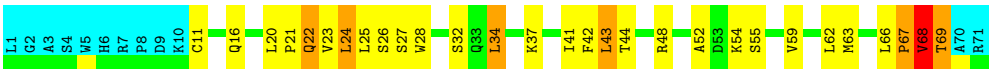
Chain A: 37% 38% 8% 17%



4.2.7 Score per residue for model 7

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

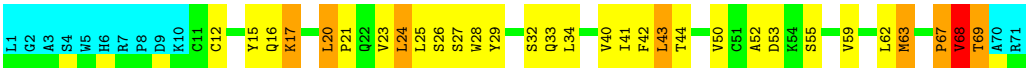
Chain A: 42% 31% 8% • 17%



4.2.8 Score per residue for model 8

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

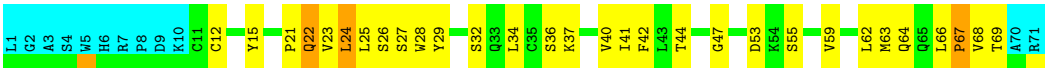
Chain A: 39% 32% 10% • 17%



4.2.9 Score per residue for model 9

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 41% 38% • 17%



4.2.10 Score per residue for model 10 (medoid)

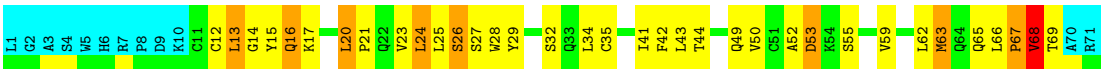
- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 37% 38% 8% 17%

4.2.11 Score per residue for model 11

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

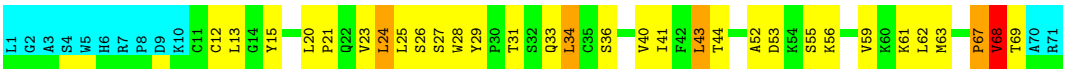
Chain A: 34% 37% 11% • 17%



4.2.12 Score per residue for model 12

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

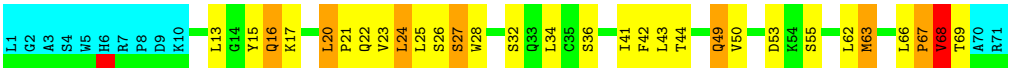
Chain A: 39% 37% 6% • 17%



4.2.13 Score per residue for model 13

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

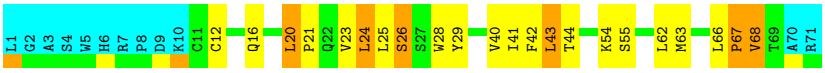
Chain A: 41% 31% 10% • 17%



4.2.14 Score per residue for model 14

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

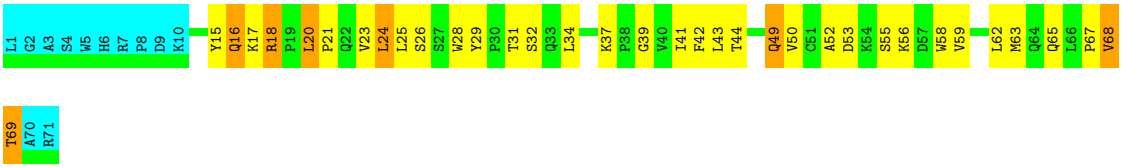
Chain A: 52% 23% 8% 17%



4.2.15 Score per residue for model 15

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 34% 39% 10% 17%



4.2.16 Score per residue for model 16

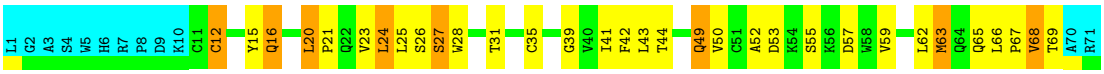
• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 41% 37% • • 17%

4.2.17 Score per residue for model 17

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

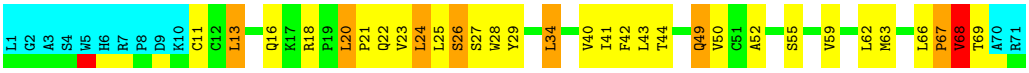
Chain A: 38% 34% 11% 17%



4.2.18 Score per residue for model 18

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

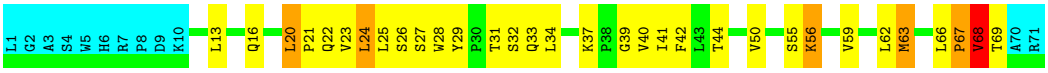
Chain A: 39% 32% 10% • 17%



4.2.19 Score per residue for model 19

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

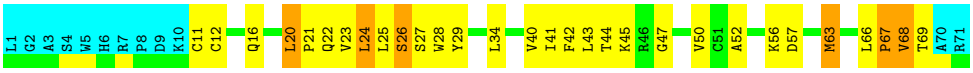
Chain A: 38% 37% 7% • 17%



4.2.20 Score per residue for model 20

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

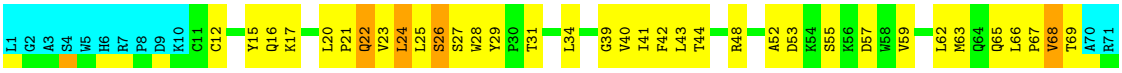
Chain A: 41% 34% 8% 17%



4.2.21 Score per residue for model 21

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 34% 44% 6% 17%



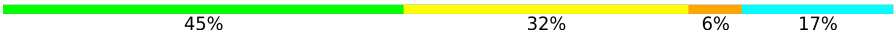
4.2.22 Score per residue for model 22

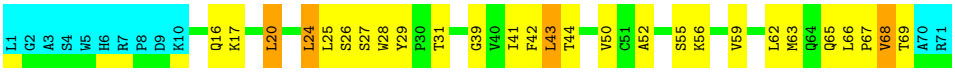
• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A: 42% 30% 11% 17%

4.2.23 Score per residue for model 23

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

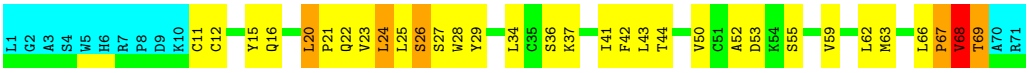
Chain A: 



4.2.24 Score per residue for model 24

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

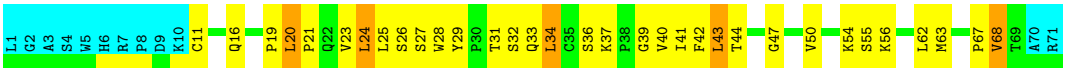
Chain A:



4.2.25 Score per residue for model 25

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

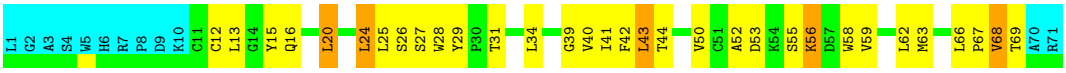
Chain A:



4.2.26 Score per residue for model 26

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

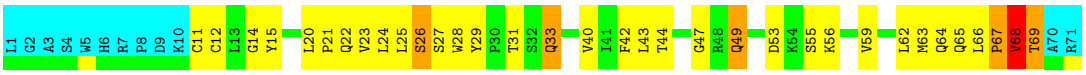
Chain A:



4.2.27 Score per residue for model 27

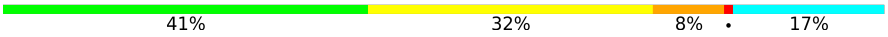
- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

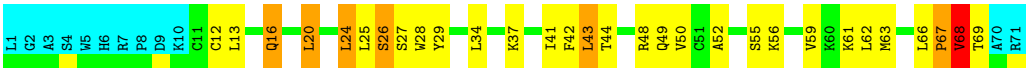
Chain A:



4.2.28 Score per residue for model 28

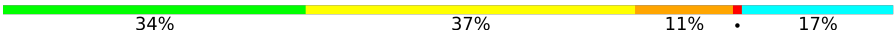
- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

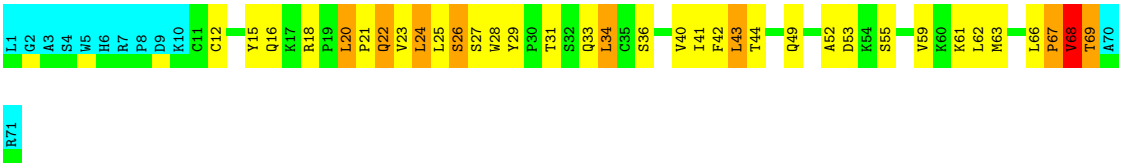
Chain A: 



4.2.29 Score per residue for model 29

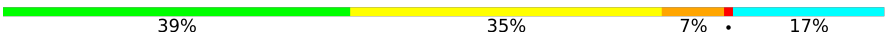
- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

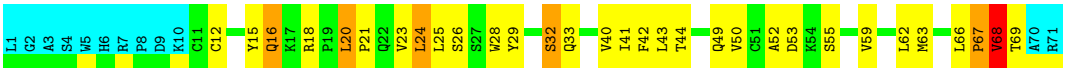
Chain A: 



4.2.30 Score per residue for model 30

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

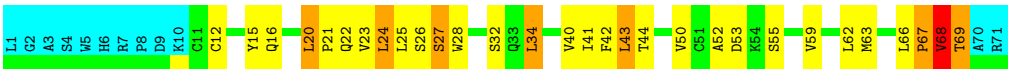
Chain A: 



4.2.31 Score per residue for model 31

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

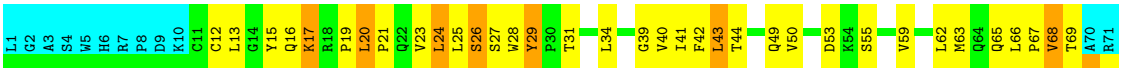
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

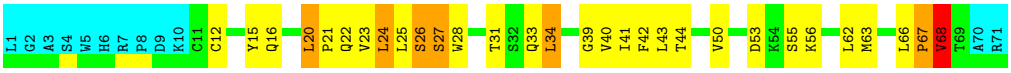
Chain A: 34% 39% 10% 17%



4.2.33 Score per residue for model 33

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

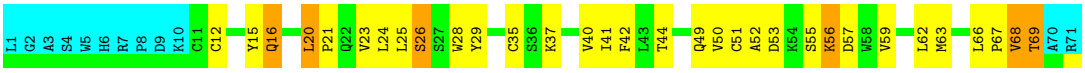
Chain A: 41% 32% 8% • 17%



4.2.34 Score per residue for model 34

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

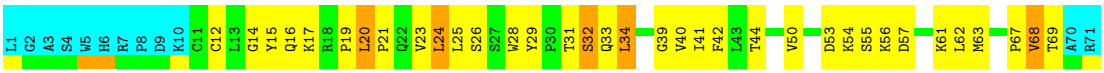
Chain A: 38% 37% 8% 17%



4.2.35 Score per residue for model 35

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

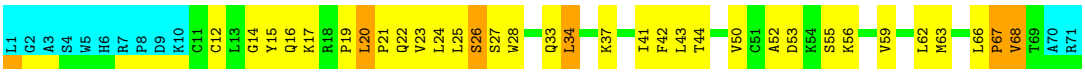
Chain A: 34% 42% 7% 17%



4.2.36 Score per residue for model 36

• Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

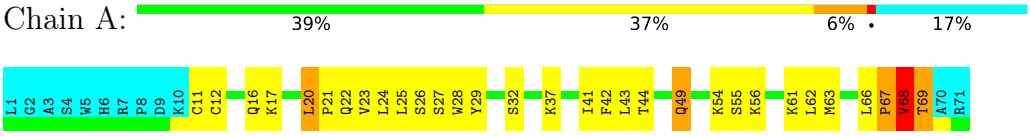
Chain A: 37% 39% 7% 17%



4.2.37 Score per residue for model 37

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

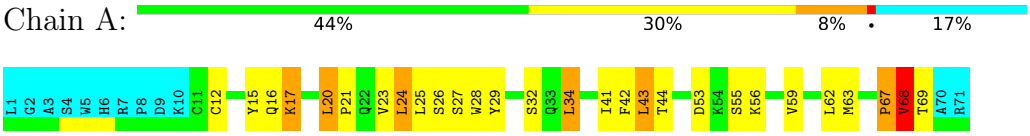
Chain A:



4.2.38 Score per residue for model 38

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 38 calculated structures, 38 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

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

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	471	497	497	27±4
All	All	17898	18886	18886	1014

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD11	1:A:50:VAL:HG11	0.85	1.49	11	6
1:A:25:LEU:HD23	1:A:62:LEU:HD22	0.81	1.52	3	33
1:A:43:LEU:HD11	1:A:69:THR:HG21	0.80	1.52	23	2
1:A:42:PHE:O	1:A:43:LEU:HD13	0.78	1.78	25	1
1:A:24:LEU:HD23	1:A:25:LEU:N	0.78	1.93	20	10
1:A:25:LEU:HD21	1:A:42:PHE:CD2	0.76	2.16	18	28
1:A:43:LEU:CD1	1:A:69:THR:HG21	0.73	2.14	37	5
1:A:28:TRP:CZ2	1:A:68:VAL:HG23	0.72	2.18	33	17
1:A:24:LEU:HD12	1:A:25:LEU:N	0.72	2.00	34	5
1:A:25:LEU:HD12	1:A:44:THR:HG22	0.71	1.60	11	36
1:A:67:PRO:O	1:A:68:VAL:HG23	0.71	1.85	9	16
1:A:16:GLN:OE1	1:A:20:LEU:HD11	0.71	1.85	25	5
1:A:20:LEU:HD11	1:A:50:VAL:HG21	0.71	1.60	15	2
1:A:43:LEU:HD23	1:A:49:GLN:CG	0.70	2.17	27	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLN:CG	1:A:66:LEU:HD21	0.70	2.17	3	11
1:A:52:ALA:HB1	1:A:59:VAL:CG1	0.70	2.17	31	6
1:A:25:LEU:CD1	1:A:44:THR:HG22	0.70	2.17	34	37
1:A:29:TYR:CE1	1:A:43:LEU:HD21	0.69	2.23	24	4
1:A:24:LEU:HD22	1:A:24:LEU:O	0.68	1.88	28	22
1:A:43:LEU:HD23	1:A:49:GLN:HG3	0.68	1.64	15	10
1:A:25:LEU:CD2	1:A:62:LEU:HD22	0.68	2.19	6	32
1:A:53:ASP:O	1:A:59:VAL:HG11	0.67	1.89	16	4
1:A:52:ALA:HB1	1:A:59:VAL:HG13	0.67	1.65	29	4
1:A:25:LEU:HD21	1:A:42:PHE:CD1	0.67	2.24	27	9
1:A:29:TYR:CD1	1:A:43:LEU:HD21	0.67	2.25	24	3
1:A:43:LEU:HD12	1:A:69:THR:HG21	0.66	1.66	1	5
1:A:16:GLN:HG2	1:A:20:LEU:HD21	0.65	1.67	21	18
1:A:31:THR:HG22	1:A:39:GLY:O	0.65	1.91	26	11
1:A:16:GLN:HG3	1:A:20:LEU:HD21	0.65	1.68	30	4
1:A:26:SER:O	1:A:66:LEU:HD22	0.65	1.91	33	13
1:A:58:TRP:O	1:A:62:LEU:HD12	0.65	1.91	22	1
1:A:29:TYR:HB3	1:A:69:THR:HG23	0.65	1.69	21	6
1:A:52:ALA:HB1	1:A:59:VAL:HG21	0.64	1.69	23	6
1:A:16:GLN:OE1	1:A:50:VAL:HG13	0.64	1.93	5	7
1:A:52:ALA:HB1	1:A:59:VAL:CG2	0.64	2.23	23	10
1:A:29:TYR:HB3	1:A:69:THR:HG22	0.64	1.70	34	1
1:A:62:LEU:O	1:A:66:LEU:HD12	0.63	1.93	30	1
1:A:21:PRO:HB2	1:A:23:VAL:HG12	0.63	1.69	34	35
1:A:16:GLN:OE1	1:A:50:VAL:HG11	0.62	1.95	25	7
1:A:34:LEU:N	1:A:34:LEU:HD13	0.62	2.10	12	5
1:A:24:LEU:O	1:A:24:LEU:HD22	0.61	1.94	7	1
1:A:32:SER:OG	1:A:34:LEU:HD11	0.61	1.96	35	1
1:A:26:SER:O	1:A:66:LEU:HD12	0.61	1.95	22	7
1:A:22:GLN:CG	1:A:66:LEU:HD11	0.61	2.26	31	1
1:A:41:ILE:HD13	1:A:50:VAL:C	0.61	2.16	18	3
1:A:29:TYR:O	1:A:40:VAL:HG13	0.60	1.96	18	18
1:A:41:ILE:HD12	1:A:49:GLN:HB3	0.60	1.72	34	3
1:A:43:LEU:HD22	1:A:43:LEU:N	0.60	2.11	26	4
1:A:34:LEU:HD22	1:A:34:LEU:N	0.60	2.12	10	17
1:A:12:CYS:C	1:A:13:LEU:HD22	0.59	2.18	26	1
1:A:41:ILE:N	1:A:41:ILE:HD12	0.58	2.12	32	32
1:A:34:LEU:HD12	1:A:34:LEU:O	0.58	1.98	15	6
1:A:42:PHE:C	1:A:43:LEU:HD13	0.58	2.18	25	1
1:A:43:LEU:HD12	1:A:43:LEU:N	0.58	2.13	29	3
1:A:27:SER:HA	1:A:66:LEU:HD23	0.58	1.76	31	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:TRP:CE3	1:A:63:MET:HE1	0.57	2.34	35	10
1:A:41:ILE:HD12	1:A:41:ILE:N	0.57	2.15	7	2
1:A:42:PHE:CE1	1:A:52:ALA:HB3	0.57	2.35	20	4
1:A:42:PHE:CZ	1:A:59:VAL:HG13	0.57	2.34	1	1
1:A:29:TYR:CD2	1:A:43:LEU:HD11	0.57	2.35	26	2
1:A:24:LEU:HD13	1:A:25:LEU:N	0.57	2.14	26	3
1:A:28:TRP:CZ3	1:A:63:MET:HE2	0.57	2.35	22	17
1:A:22:GLN:HG3	1:A:66:LEU:HD21	0.56	1.76	1	3
1:A:12:CYS:SG	1:A:41:ILE:HD11	0.56	2.41	22	9
1:A:29:TYR:CB	1:A:69:THR:HG22	0.56	2.30	34	1
1:A:42:PHE:CE1	1:A:59:VAL:HG13	0.56	2.36	36	9
1:A:29:TYR:CE1	1:A:43:LEU:HD11	0.55	2.36	25	1
1:A:24:LEU:HD23	1:A:25:LEU:H	0.55	1.61	3	9
1:A:33:GLN:O	1:A:34:LEU:HD13	0.55	2.02	1	2
1:A:22:GLN:HG3	1:A:66:LEU:HD11	0.55	1.79	19	3
1:A:59:VAL:HA	1:A:62:LEU:HD12	0.54	1.78	28	8
1:A:29:TYR:CD1	1:A:43:LEU:HD11	0.54	2.37	25	6
1:A:13:LEU:N	1:A:13:LEU:HD22	0.54	2.17	10	2
1:A:16:GLN:CG	1:A:50:VAL:HG11	0.53	2.32	30	2
1:A:13:LEU:O	1:A:13:LEU:HD23	0.53	2.04	11	2
1:A:25:LEU:HD12	1:A:44:THR:HA	0.53	1.79	9	3
1:A:69:THR:HG23	1:A:69:THR:O	0.53	2.04	1	2
1:A:29:TYR:CE2	1:A:43:LEU:HD11	0.53	2.39	14	2
1:A:43:LEU:HD13	1:A:69:THR:HG21	0.52	1.81	12	1
1:A:42:PHE:CE2	1:A:59:VAL:HG13	0.52	2.39	38	4
1:A:20:LEU:N	1:A:20:LEU:HD23	0.52	2.20	1	21
1:A:24:LEU:HD22	1:A:24:LEU:C	0.52	2.26	21	23
1:A:16:GLN:HE21	1:A:50:VAL:HG13	0.52	1.65	23	1
1:A:41:ILE:HD11	1:A:51:CYS:SG	0.51	2.44	34	1
1:A:16:GLN:CG	1:A:20:LEU:HD21	0.51	2.35	35	8
1:A:43:LEU:HD12	1:A:69:THR:CG2	0.51	2.35	10	2
1:A:24:LEU:HD12	1:A:24:LEU:C	0.51	2.26	27	5
1:A:42:PHE:HE2	1:A:59:VAL:HG13	0.51	1.65	9	3
1:A:13:LEU:HD12	1:A:13:LEU:N	0.51	2.21	28	2
1:A:29:TYR:C	1:A:40:VAL:HG13	0.51	2.27	9	3
1:A:22:GLN:HG2	1:A:66:LEU:HD21	0.51	1.82	20	3
1:A:31:THR:HG23	1:A:41:ILE:CD1	0.50	2.36	6	1
1:A:16:GLN:CG	1:A:50:VAL:HG13	0.50	2.36	11	4
1:A:20:LEU:HD11	1:A:50:VAL:CG1	0.50	2.31	11	1
1:A:16:GLN:NE2	1:A:58:TRP:CZ2	0.50	2.80	15	1
1:A:24:LEU:HD13	1:A:24:LEU:C	0.50	2.27	28	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:TRP:CZ3	1:A:68:VAL:HG23	0.49	2.42	32	1
1:A:27:SER:CA	1:A:66:LEU:HD23	0.49	2.37	31	3
1:A:16:GLN:NE2	1:A:50:VAL:HG13	0.49	2.22	4	2
1:A:43:LEU:HD11	1:A:69:THR:CG2	0.49	2.32	23	2
1:A:58:TRP:CE2	1:A:59:VAL:HG23	0.49	2.42	15	2
1:A:67:PRO:O	1:A:68:VAL:HG12	0.49	2.08	22	2
1:A:33:GLN:C	1:A:34:LEU:HD13	0.49	2.28	1	5
1:A:43:LEU:HD23	1:A:49:GLN:HG2	0.48	1.83	30	2
1:A:22:GLN:HG2	1:A:66:LEU:HD11	0.48	1.85	31	1
1:A:28:TRP:CZ3	1:A:63:MET:HE1	0.48	2.44	35	5
1:A:16:GLN:OE1	1:A:20:LEU:HD21	0.48	2.09	34	2
1:A:25:LEU:HD13	1:A:44:THR:HG22	0.47	1.84	20	1
1:A:66:LEU:N	1:A:66:LEU:HD12	0.47	2.24	13	4
1:A:28:TRP:C	1:A:69:THR:HG22	0.47	2.30	21	1
1:A:28:TRP:CH2	1:A:68:VAL:CG2	0.46	2.99	8	14
1:A:28:TRP:CE3	1:A:63:MET:CE	0.46	2.99	29	10
1:A:67:PRO:O	1:A:68:VAL:CB	0.46	2.64	20	2
1:A:28:TRP:HA	1:A:43:LEU:HD23	0.46	1.88	28	1
1:A:28:TRP:CZ2	1:A:68:VAL:CG2	0.46	2.99	12	12
1:A:42:PHE:HE1	1:A:52:ALA:HB3	0.45	1.70	20	1
1:A:52:ALA:CB	1:A:59:VAL:HG13	0.45	2.41	21	2
1:A:25:LEU:CD2	1:A:42:PHE:CD2	0.45	2.99	23	6
1:A:28:TRP:CH2	1:A:68:VAL:HG23	0.45	2.46	28	5
1:A:65:GLN:C	1:A:66:LEU:HD12	0.45	2.32	17	1
1:A:19:PRO:C	1:A:20:LEU:HD23	0.45	2.32	32	6
1:A:28:TRP:CZ3	1:A:63:MET:CE	0.45	3.00	13	22
1:A:16:GLN:HG3	1:A:50:VAL:HG13	0.45	1.86	34	1
1:A:28:TRP:CE3	1:A:63:MET:HE2	0.45	2.47	34	16
1:A:20:LEU:CD1	1:A:50:VAL:HG21	0.45	2.42	34	1
1:A:42:PHE:CE2	1:A:52:ALA:HB2	0.44	2.47	30	1
1:A:27:SER:HA	1:A:66:LEU:HD13	0.44	1.87	33	1
1:A:20:LEU:HD23	1:A:20:LEU:N	0.44	2.27	32	1
1:A:12:CYS:O	1:A:13:LEU:HD22	0.43	2.13	26	1
1:A:25:LEU:HD12	1:A:44:THR:CG2	0.43	2.41	34	2
1:A:66:LEU:HD12	1:A:66:LEU:N	0.43	2.28	17	1
1:A:16:GLN:OE1	1:A:58:TRP:CH2	0.43	2.71	15	1
1:A:16:GLN:NE2	1:A:20:LEU:HD21	0.43	2.28	33	2
1:A:29:TYR:CE1	1:A:41:ILE:CG2	0.43	3.02	28	5
1:A:25:LEU:HD21	1:A:42:PHE:HD2	0.42	1.74	1	1
1:A:15:TYR:CD1	1:A:15:TYR:N	0.42	2.87	3	1
1:A:23:VAL:HG13	1:A:24:LEU:N	0.42	2.30	6	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:TRP:CH2	1:A:63:MET:HE2	0.42	2.49	22	1
1:A:25:LEU:HD11	1:A:42:PHE:HB3	0.42	1.91	6	5
1:A:34:LEU:N	1:A:34:LEU:CD1	0.42	2.82	33	3
1:A:33:GLN:N	1:A:34:LEU:HD13	0.42	2.29	35	2
1:A:13:LEU:HD23	1:A:13:LEU:N	0.42	2.29	18	1
1:A:34:LEU:N	1:A:34:LEU:CD2	0.42	2.83	31	2
1:A:28:TRP:CE3	1:A:68:VAL:HG23	0.42	2.49	20	2
1:A:43:LEU:HD22	1:A:43:LEU:H	0.42	1.73	32	1
1:A:66:LEU:HD22	1:A:66:LEU:N	0.42	2.29	6	1
1:A:42:PHE:CZ	1:A:62:LEU:HD13	0.42	2.50	30	1
1:A:43:LEU:N	1:A:43:LEU:CD2	0.42	2.83	25	3
1:A:16:GLN:HG2	1:A:50:VAL:HG13	0.41	1.91	11	1
1:A:67:PRO:O	1:A:68:VAL:CG2	0.41	2.68	27	1
1:A:43:LEU:HD21	1:A:69:THR:HG23	0.41	1.91	31	1
1:A:28:TRP:CE2	1:A:68:VAL:HG23	0.41	2.50	13	1
1:A:15:TYR:CZ	1:A:53:ASP:OD2	0.41	2.74	35	13
1:A:16:GLN:O	1:A:17:LYS:CB	0.41	2.68	8	4
1:A:28:TRP:O	1:A:68:VAL:HG22	0.41	2.16	30	1
1:A:16:GLN:NE2	1:A:18:ARG:N	0.41	2.69	15	1
1:A:35:CYS:O	1:A:37:LYS:N	0.41	2.54	22	1
1:A:15:TYR:CE2	1:A:53:ASP:OD2	0.41	2.74	27	7
1:A:41:ILE:N	1:A:41:ILE:CD1	0.41	2.83	3	5
1:A:28:TRP:CZ2	1:A:67:PRO:O	0.41	2.74	36	11
1:A:14:GLY:O	1:A:15:TYR:CG	0.41	2.74	11	5
1:A:28:TRP:CE3	1:A:40:VAL:HG11	0.41	2.51	33	4
1:A:66:LEU:N	1:A:66:LEU:CD1	0.41	2.83	17	2
1:A:36:SER:OG	1:A:37:LYS:N	0.41	2.54	24	1
1:A:42:PHE:HE2	1:A:66:LEU:HD12	0.41	1.75	34	1
1:A:29:TYR:HB2	1:A:69:THR:HG21	0.41	1.92	9	1
1:A:68:VAL:CG1	1:A:69:THR:N	0.41	2.84	9	2
1:A:15:TYR:CD2	1:A:53:ASP:OD2	0.41	2.74	11	1
1:A:11:CYS:HA	1:A:31:THR:HG22	0.41	1.93	27	1
1:A:15:TYR:CE1	1:A:53:ASP:OD2	0.41	2.74	5	6
1:A:13:LEU:N	1:A:13:LEU:CD2	0.41	2.84	10	1
1:A:15:TYR:CZ	1:A:53:ASP:OD1	0.41	2.74	13	4
1:A:15:TYR:CD1	1:A:53:ASP:OD2	0.41	2.74	21	3
1:A:44:THR:HG23	1:A:48:ARG:O	0.40	2.16	28	1
1:A:29:TYR:HB3	1:A:69:THR:HG21	0.40	1.94	24	2
1:A:14:GLY:O	1:A:15:TYR:CD1	0.40	2.74	36	1
1:A:29:TYR:CB	1:A:69:THR:CG2	0.40	2.99	9	1
1:A:29:TYR:CD1	1:A:43:LEU:CD1	0.40	3.05	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLN:NE2	1:A:66:LEU:HD21	0.40	2.31	18	1
1:A:43:LEU:CD1	1:A:69:THR:CG2	0.40	2.99	27	2
1:A:52:ALA:HB1	1:A:59:VAL:HG11	0.40	1.89	31	1
1:A:42:PHE:O	1:A:43:LEU:HD12	0.40	2.17	21	1
1:A:41:ILE:CG2	1:A:49:GLN:CG	0.40	2.99	34	1
1:A:29:TYR:CB	1:A:69:THR:HG21	0.40	2.46	9	1
1:A:28:TRP:CD1	1:A:42:PHE:CE2	0.40	3.09	28	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	59/71 (83%)	49±2 (83±4%)	6±2 (10±3%)	4±1 (7±2%)	2 18
All	All	2242/2698 (83%)	1862 (83%)	231 (10%)	149 (7%)	2 18

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	A	67	PRO	38
1	A	68	VAL	37
1	A	56	LYS	22
1	A	12	CYS	13
1	A	11	CYS	10
1	A	17	LYS	10
1	A	47	GLY	4
1	A	36	SER	4
1	A	33	GLN	3
1	A	35	CYS	3
1	A	32	SER	2
1	A	69	THR	2
1	A	34	LEU	1

6.3.2 Protein sidechains (i)

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	55/64 (86%)	45±2 (82±3%)	10±2 (18±3%)	4 38
All	All	2090/2432 (86%)	1714 (82%)	376 (18%)	4 38

All 32 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	55	SER	37
1	A	68	VAL	34
1	A	20	LEU	33
1	A	24	LEU	33
1	A	26	SER	32
1	A	27	SER	25
1	A	69	THR	19
1	A	32	SER	17
1	A	43	LEU	16
1	A	34	LEU	14
1	A	63	MET	13
1	A	37	LYS	11
1	A	54	LYS	9
1	A	49	GLN	9
1	A	57	ASP	8
1	A	65	GLN	8
1	A	61	LYS	7
1	A	22	GLN	7
1	A	16	GLN	7
1	A	31	THR	4
1	A	17	LYS	4
1	A	36	SER	4
1	A	13	LEU	4
1	A	18	ARG	4
1	A	56	LYS	4
1	A	33	GLN	3
1	A	12	CYS	3
1	A	48	ARG	2
1	A	64	GLN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	53	ASP	1
1	A	45	LYS	1
1	A	29	TYR	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 (i)

No chemical shift data were provided