Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 04:50 PM EST

PDB ID	:	1R6P
Title	:	NMR structure of the N-terminal domain of trout cardiac troponin C at 7 C
Authors	:	Blumenschein, T.M.; Gillis, T.E.; Tibbits, G.F.; Sykes, B.D.
Deposited on	:	2003-10-15

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

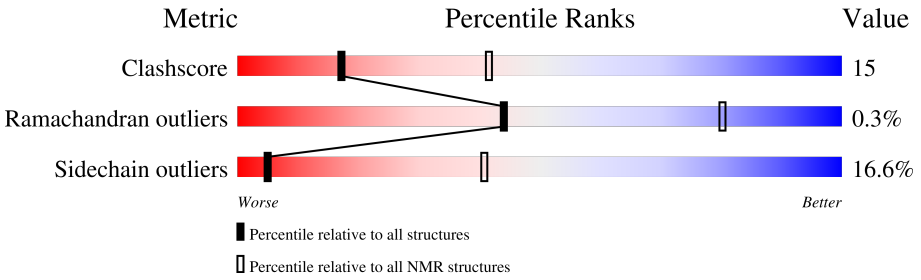
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	89	61% 27% • 11%

2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 27 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:5-A:83 (79)	0.41	27

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 8 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 4, 6, 8, 17, 19, 21, 22, 24, 25, 26, 27, 31, 32, 33, 36, 38, 39, 40
2	5, 9, 14, 30, 35, 37
3	1, 16, 23
4	2, 13, 20
5	7, 29
6	11, 28
7	18, 34
8	10, 15
Single-model clusters	12

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1370 atoms, of which 666 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called troponin C.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1369	433	666	109	152	9	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	1	1	1

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: troponin C

Chain A: 61% 27% • 11%

M1 N2 D3 I4 Y5 K6 L12 T13 Q16 F20 K21 F24 F27 I28 I36 S37 T38 L41 V44 L48 T53 P54 L57 I61 V64 D65 V72 F77 L78 V79 V82 R83 C84 M85 K86 D87 D88 S89

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: troponin C

Chain A: 64% 22% • 11%

M1 N2 D3 I4 Y5 K6 V9 L12 T13 F20 K21 F27 I28 A31 S37 T38 L41 V44 M45 T53 P54 I61 D65 E66 D67 F74 F77 L78 C84 M85 K86 D87 D88 S89

4.2.2 Score per residue for model 2

• Molecule 1: troponin C

Chain A: 54% 30% • 11%

M1 N2 D3 I4 Y5 K6 L12 T13 Q16 K17 F20 F24 D25 I26 F27 I28 E32 C35 I36 S37 T38 L41 V44 Q50 T53 P54 I61 V64 D65 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

4.2.3 Score per residue for model 3

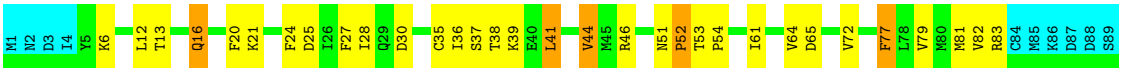
- Molecule 1: troponin C

Chain A: 64% 24% • 11%

4.2.4 Score per residue for model 4

- Molecule 1: troponin C

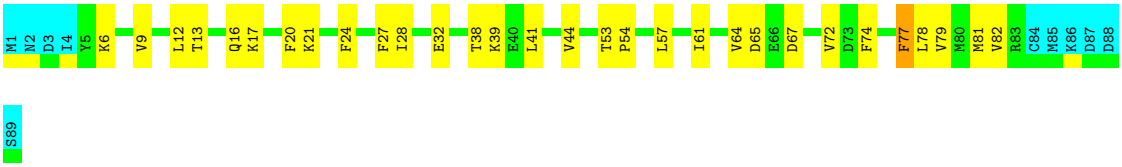
Chain A: 53% 30% 6% 11%



4.2.5 Score per residue for model 5

- Molecule 1: troponin C

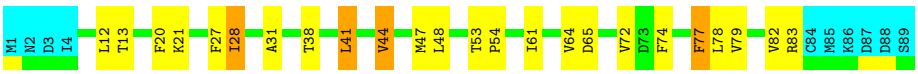
Chain A: 55% 33% • 11%



4.2.6 Score per residue for model 6

- Molecule 1: troponin C

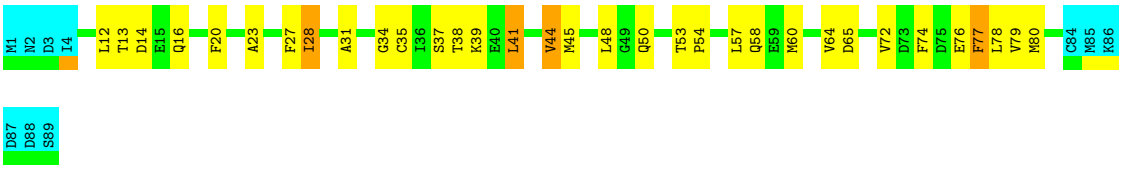
Chain A: 62% 22% • 11%



4.2.7 Score per residue for model 7

- Molecule 1: troponin C

Chain A: 52% 33% • 11%



4.2.8 Score per residue for model 8

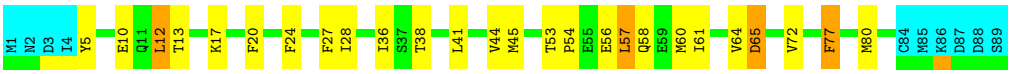
- Molecule 1: troponin C

Chain A: 55% 29% • 11%

4.2.9 Score per residue for model 9

- Molecule 1: troponin C

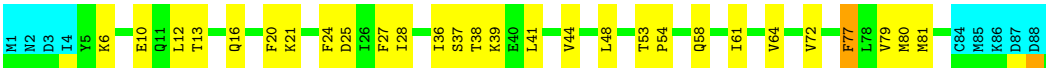
Chain A: 60% 25% • 11%



4.2.10 Score per residue for model 10

- Molecule 1: troponin C

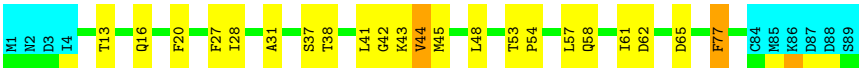
Chain A: 57% 30% • 11%



4.2.11 Score per residue for model 11

- Molecule 1: troponin C

Chain A: 64% 22% • 11%



4.2.12 Score per residue for model 12

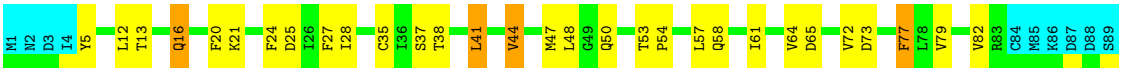
- Molecule 1: troponin C

Chain A: 57% 28% • 11%

4.2.13 Score per residue for model 13

- Molecule 1: troponin C

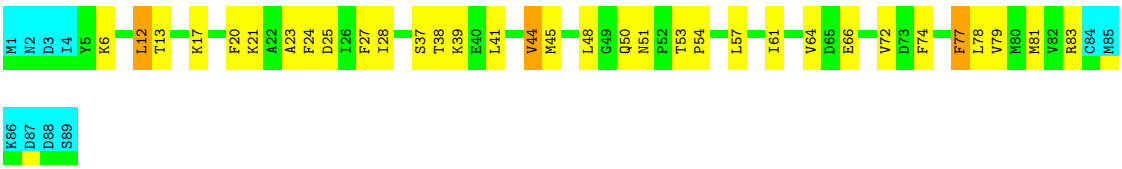
Chain A: 55% 29% • 11%



4.2.14 Score per residue for model 14

- Molecule 1: troponin C

Chain A: 52% 34% • 11%



4.2.15 Score per residue for model 15

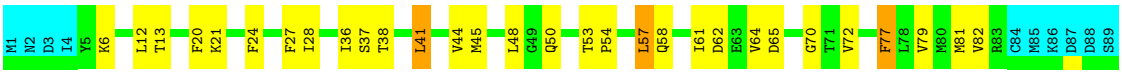
- Molecule 1: troponin C

Chain A: 64% 24% • 11%

4.2.16 Score per residue for model 16

- Molecule 1: troponin C

Chain A: 55% 30% • 11%



4.2.17 Score per residue for model 17

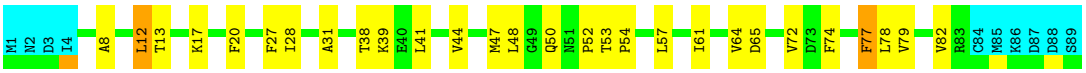
- Molecule 1: troponin C

Chain A: 57% 29% • 11%

4.2.18 Score per residue for model 18

- Molecule 1: troponin C

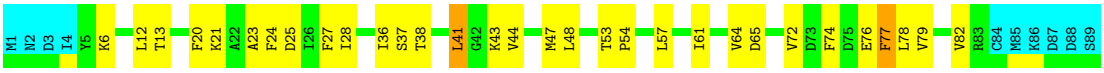
Chain A: 57% 29% • 11%



4.2.19 Score per residue for model 19

- Molecule 1: troponin C

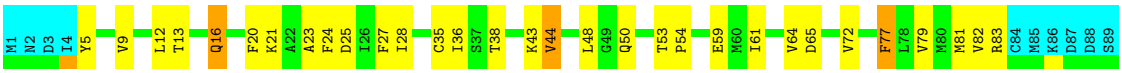
Chain A: 54% 33% • 11%



4.2.20 Score per residue for model 20

- Molecule 1: troponin C

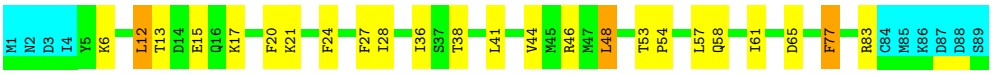
Chain A: 54% 31% • 11%



4.2.21 Score per residue for model 21

- Molecule 1: troponin C

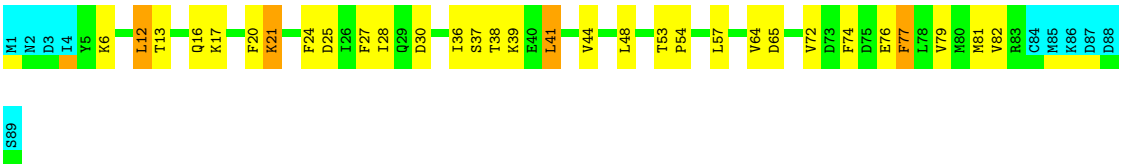
Chain A: 62% 24% • 11%



4.2.22 Score per residue for model 22

- Molecule 1: troponin C

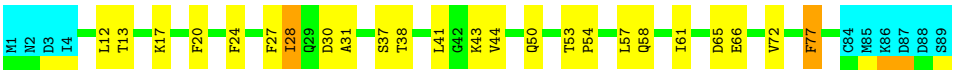
Chain A: 54% 30% • 11%



4.2.23 Score per residue for model 23

- Molecule 1: troponin C

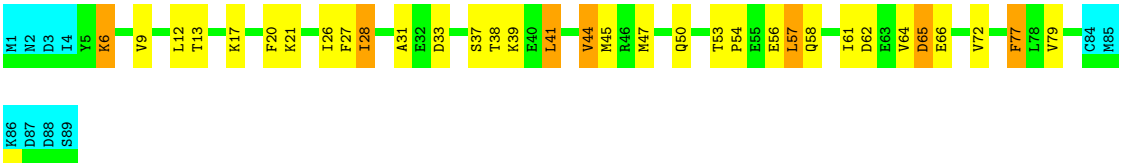
Chain A: 62% 25% • 11%



4.2.24 Score per residue for model 24

- Molecule 1: troponin C

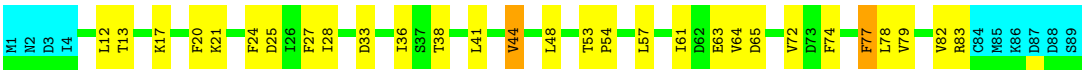
Chain A: 52% 29% 8% 11%



4.2.25 Score per residue for model 25

- Molecule 1: troponin C

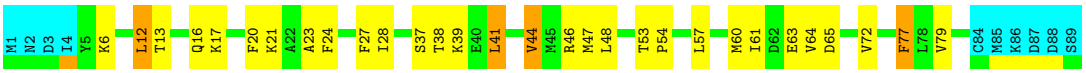
Chain A: 56% 30% • 11%



4.2.26 Score per residue for model 26

- Molecule 1: troponin C

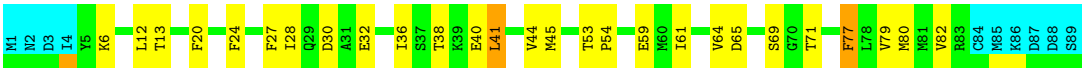
Chain A: 55% 29% • 11%



4.2.27 Score per residue for model 27 (medoid)

- Molecule 1: troponin C

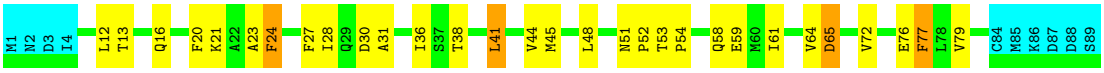
Chain A: 58% 28% • 11%



4.2.28 Score per residue for model 28

- Molecule 1: troponin C

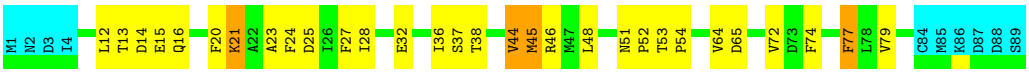
Chain A: 55% 29% • 11%



4.2.29 Score per residue for model 29

- Molecule 1: troponin C

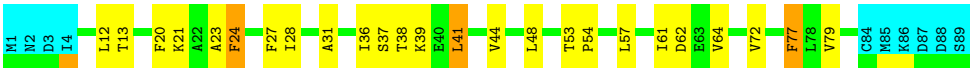
Chain A: 55% 29% • 11%



4.2.30 Score per residue for model 30

- Molecule 1: troponin C

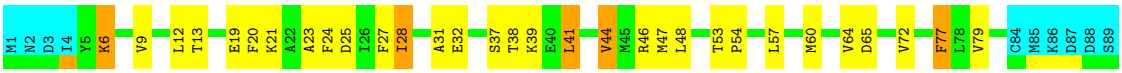
Chain A: 61% 25% • 11%



4.2.31 Score per residue for model 31

- Molecule 1: troponin C

Chain A: 54% 29% 6% 11%



4.2.32 Score per residue for model 32

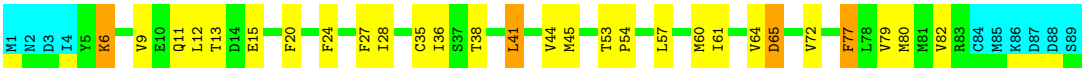
- Molecule 1: troponin C

Chain A: 62% 24% • 11%

4.2.33 Score per residue for model 33

- Molecule 1: troponin C

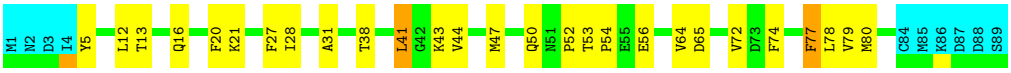
Chain A: 57% 27% • 11%



4.2.34 Score per residue for model 34

- Molecule 1: troponin C

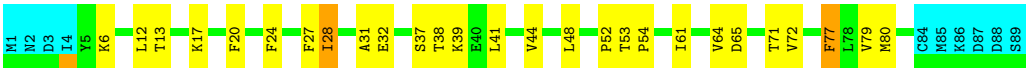
Chain A: 58% 28% • 11%



4.2.35 Score per residue for model 35

- Molecule 1: troponin C

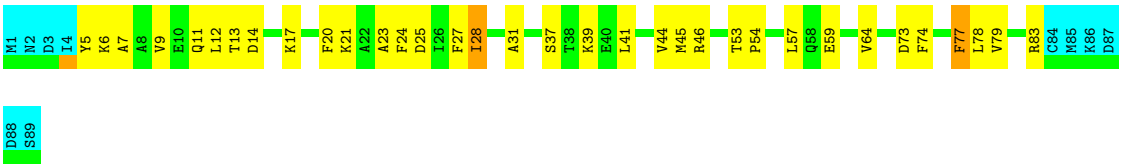
Chain A: 58% 28% • 11%



4.2.36 Score per residue for model 36

- Molecule 1: troponin C

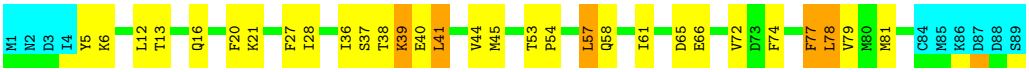
Chain A: 51% 36% • 11%



4.2.37 Score per residue for model 37

- Molecule 1: troponin C

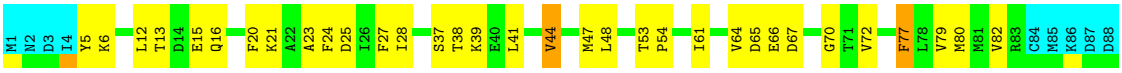
Chain A: 55% 28% 6% 11%



4.2.38 Score per residue for model 38

- Molecule 1: troponin C

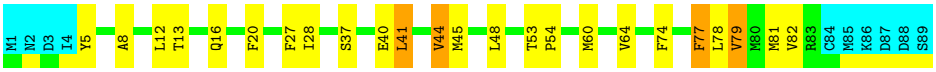
Chain A: 52% 35% • 11%



4.2.39 Score per residue for model 39

- Molecule 1: troponin C

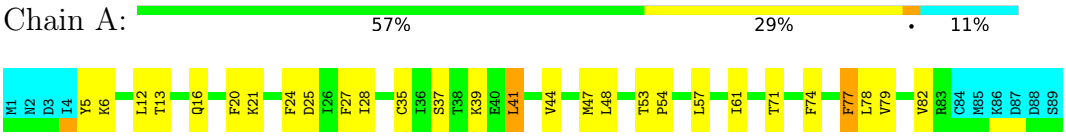
Chain A: 62% 22% • 11%



4.2.40 Score per residue for model 40

- Molecule 1: troponin C

Chain A:


57%
29%
11%
M1 N2 D3 I4 Y5 K6 L12 T13 Q16 F20 K21 F24 D25 I26 F27 I28 C35 I36 S37 T38 K39 E40 L41 V44 M47 L48 T53 P54 L57 I61 T71 F74 F77 L78 V79 V82 R83 C84 M85 K86 D87 D88 S89

5 Refinement protocol and experimental data overview (i)

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

Of the 60 calculated structures, 40 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	refinement	3.851

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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	625	594	594	19±4
All	All	25040	23760	23760	748

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HG23	1:A:31:ALA:HB3	0.97	1.36	18	3
1:A:27:PHE:CE2	1:A:44:VAL:HG22	0.80	2.11	16	18
1:A:41:LEU:HD13	1:A:61:ILE:HD11	0.80	1.51	14	5
1:A:27:PHE:CE2	1:A:44:VAL:HG12	0.80	2.12	25	19
1:A:41:LEU:HD12	1:A:44:VAL:CG1	0.75	2.11	35	1
1:A:64:VAL:HG13	1:A:79:VAL:CG1	0.73	2.13	39	4
1:A:44:VAL:HG21	1:A:77:PHE:HZ	0.72	1.44	35	2
1:A:38:THR:HB	1:A:61:ILE:HG21	0.71	1.61	1	15
1:A:41:LEU:HD13	1:A:61:ILE:HG12	0.71	1.62	25	2
1:A:24:PHE:CE1	1:A:28:ILE:HG21	0.70	2.21	13	21
1:A:38:THR:OG1	1:A:61:ILE:HG21	0.70	1.86	3	3
1:A:44:VAL:HG11	1:A:77:PHE:CE1	0.69	2.22	30	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:HG23	1:A:79:VAL:CG1	0.69	2.18	28	24
1:A:20:PHE:CE1	1:A:48:LEU:HD21	0.69	2.22	40	10
1:A:28:ILE:HG23	1:A:31:ALA:CB	0.68	2.17	18	3
1:A:20:PHE:CE2	1:A:48:LEU:HD21	0.67	2.24	20	6
1:A:64:VAL:HG21	1:A:80:MET:HG3	0.67	1.66	9	1
1:A:44:VAL:HG21	1:A:77:PHE:CZ	0.67	2.24	34	2
1:A:38:THR:HB	1:A:61:ILE:HD13	0.67	1.65	6	10
1:A:41:LEU:HB3	1:A:57:LEU:HD21	0.66	1.68	9	1
1:A:41:LEU:HD12	1:A:72:VAL:HG21	0.66	1.68	25	3
1:A:28:ILE:O	1:A:28:ILE:HG23	0.66	1.90	28	5
1:A:28:ILE:HG23	1:A:28:ILE:O	0.64	1.92	1	7
1:A:44:VAL:HG11	1:A:77:PHE:CZ	0.64	2.27	15	15
1:A:41:LEU:HD22	1:A:61:ILE:HD11	0.64	1.68	9	1
1:A:74:PHE:O	1:A:78:LEU:HD22	0.63	1.94	37	1
1:A:41:LEU:HB2	1:A:61:ILE:HD11	0.62	1.72	17	3
1:A:44:VAL:HG11	1:A:77:PHE:HZ	0.62	1.53	16	5
1:A:12:LEU:CD2	1:A:78:LEU:HD23	0.62	2.24	14	2
1:A:57:LEU:HD13	1:A:58:GLN:N	0.62	2.10	24	5
1:A:28:ILE:HG13	1:A:31:ALA:HB2	0.62	1.72	28	1
1:A:28:ILE:HG22	1:A:28:ILE:O	0.61	1.95	11	2
1:A:64:VAL:HG23	1:A:79:VAL:HG11	0.61	1.72	3	5
1:A:41:LEU:HD12	1:A:61:ILE:CG1	0.60	2.25	32	1
1:A:41:LEU:HD21	1:A:72:VAL:HG21	0.60	1.73	30	4
1:A:38:THR:HG22	1:A:72:VAL:CG2	0.60	2.27	18	29
1:A:74:PHE:CE2	1:A:78:LEU:HD21	0.60	2.31	37	1
1:A:28:ILE:HD12	1:A:28:ILE:O	0.60	1.97	37	25
1:A:36:ILE:HD11	1:A:41:LEU:HD22	0.59	1.75	30	4
1:A:41:LEU:HD13	1:A:61:ILE:CD1	0.59	2.28	26	4
1:A:41:LEU:HD13	1:A:44:VAL:HB	0.59	1.73	17	2
1:A:28:ILE:CD1	1:A:31:ALA:HB3	0.59	2.28	35	11
1:A:41:LEU:HD13	1:A:44:VAL:HG22	0.59	1.74	19	4
1:A:20:PHE:HB3	1:A:77:PHE:CD2	0.59	2.32	19	39
1:A:45:MET:SD	1:A:57:LEU:HD23	0.58	2.38	37	2
1:A:23:ALA:HB1	1:A:27:PHE:CE2	0.58	2.33	26	10
1:A:38:THR:HG22	1:A:72:VAL:HG23	0.58	1.75	18	11
1:A:64:VAL:HG13	1:A:79:VAL:HG12	0.58	1.74	39	3
1:A:28:ILE:HG23	1:A:36:ILE:HG22	0.58	1.75	21	10
1:A:41:LEU:HD23	1:A:44:VAL:HG22	0.58	1.75	6	2
1:A:28:ILE:O	1:A:28:ILE:HG22	0.58	1.98	34	1
1:A:41:LEU:O	1:A:41:LEU:HD13	0.58	1.98	4	8
1:A:57:LEU:O	1:A:57:LEU:HD22	0.57	1.99	24	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:HG21	1:A:77:PHE:CE1	0.57	2.34	11	16
1:A:26:ILE:HD11	1:A:47:MET:CE	0.57	2.29	24	1
1:A:57:LEU:HD13	1:A:57:LEU:C	0.57	2.19	16	5
1:A:41:LEU:CB	1:A:61:ILE:HD11	0.56	2.31	17	3
1:A:45:MET:SD	1:A:52:PRO:HD2	0.56	2.41	29	2
1:A:41:LEU:HB3	1:A:57:LEU:HD13	0.56	1.77	11	3
1:A:38:THR:OG1	1:A:61:ILE:HD13	0.56	2.00	3	1
1:A:41:LEU:HD13	1:A:61:ILE:CG1	0.56	2.29	25	2
1:A:64:VAL:HG23	1:A:79:VAL:HG12	0.55	1.79	18	17
1:A:41:LEU:HG	1:A:61:ILE:HD11	0.55	1.77	40	2
1:A:44:VAL:O	1:A:48:LEU:HD13	0.55	2.02	7	9
1:A:20:PHE:CE1	1:A:81:MET:HG2	0.54	2.37	22	2
1:A:28:ILE:HG22	1:A:35:CYS:C	0.54	2.23	13	5
1:A:12:LEU:HD13	1:A:16:GLN:HG2	0.54	1.79	13	1
1:A:53:THR:HB	1:A:54:PRO:HD2	0.54	1.80	4	40
1:A:36:ILE:HD11	1:A:41:LEU:CD2	0.52	2.34	17	4
1:A:64:VAL:HG21	1:A:76:GLU:O	0.52	2.04	19	5
1:A:38:THR:CB	1:A:61:ILE:HG21	0.52	2.31	1	5
1:A:28:ILE:HG13	1:A:31:ALA:CB	0.52	2.34	28	1
1:A:8:ALA:CB	1:A:82:VAL:HG11	0.52	2.35	17	2
1:A:28:ILE:HD13	1:A:31:ALA:HB3	0.51	1.82	23	9
1:A:41:LEU:CD2	1:A:61:ILE:HD11	0.51	2.36	9	1
1:A:12:LEU:HD13	1:A:16:GLN:HE21	0.51	1.65	4	1
1:A:41:LEU:CD1	1:A:72:VAL:HG21	0.51	2.36	16	3
1:A:27:PHE:CE2	1:A:44:VAL:HB	0.51	2.40	35	2
1:A:27:PHE:CZ	1:A:44:VAL:HG22	0.51	2.41	9	2
1:A:79:VAL:O	1:A:82:VAL:HG22	0.51	2.06	38	18
1:A:20:PHE:CZ	1:A:48:LEU:HD21	0.50	2.42	11	1
1:A:44:VAL:HG21	1:A:77:PHE:HE1	0.50	1.65	25	9
1:A:9:VAL:O	1:A:12:LEU:HD23	0.50	2.05	12	1
1:A:17:LYS:HD3	1:A:78:LEU:HD21	0.50	1.82	25	2
1:A:28:ILE:CG2	1:A:31:ALA:HB3	0.50	2.25	18	2
1:A:41:LEU:HD12	1:A:61:ILE:HG12	0.49	1.84	32	1
1:A:41:LEU:HD23	1:A:45:MET:HG3	0.49	1.84	37	1
1:A:24:PHE:O	1:A:28:ILE:HG22	0.49	2.08	30	6
1:A:64:VAL:HG23	1:A:83:ARG:HD2	0.49	1.83	25	1
1:A:36:ILE:HD11	1:A:41:LEU:HD12	0.49	1.85	37	2
1:A:41:LEU:HD21	1:A:80:MET:SD	0.49	2.48	10	1
1:A:38:THR:CG2	1:A:61:ILE:HG21	0.49	2.38	23	3
1:A:57:LEU:HD12	1:A:57:LEU:C	0.48	2.28	14	11
1:A:12:LEU:HD13	1:A:17:LYS:HD2	0.48	1.84	26	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD13	1:A:17:LYS:HG3	0.48	1.85	5	2
1:A:64:VAL:HG21	1:A:80:MET:CG	0.48	2.39	33	1
1:A:38:THR:HA	1:A:41:LEU:HD23	0.48	1.86	22	3
1:A:57:LEU:HD12	1:A:58:GLN:N	0.48	2.24	13	5
1:A:58:GLN:HA	1:A:61:ILE:HD12	0.48	1.84	21	4
1:A:60:MET:O	1:A:64:VAL:HG12	0.48	2.08	32	2
1:A:44:VAL:HG12	1:A:48:LEU:CD2	0.48	2.39	21	1
1:A:60:MET:O	1:A:64:VAL:HG23	0.47	2.09	26	4
1:A:28:ILE:O	1:A:28:ILE:CG2	0.47	2.62	7	12
1:A:74:PHE:CZ	1:A:78:LEU:HD11	0.47	2.45	1	3
1:A:19:GLU:HG2	1:A:48:LEU:CD1	0.47	2.40	31	1
1:A:20:PHE:CE1	1:A:81:MET:HB2	0.47	2.45	37	3
1:A:74:PHE:CE1	1:A:78:LEU:HD11	0.46	2.46	14	8
1:A:12:LEU:CD1	1:A:17:LYS:HG3	0.46	2.41	5	1
1:A:41:LEU:HD12	1:A:44:VAL:HB	0.46	1.85	9	1
1:A:64:VAL:HG11	1:A:80:MET:HG3	0.46	1.88	27	1
1:A:57:LEU:O	1:A:61:ILE:HD12	0.46	2.11	3	1
1:A:9:VAL:HA	1:A:12:LEU:HD23	0.46	1.87	5	1
1:A:41:LEU:CB	1:A:57:LEU:HD13	0.46	2.41	11	3
1:A:38:THR:HG22	1:A:70:GLY:C	0.45	2.31	38	3
1:A:51:ASN:N	1:A:52:PRO:HD3	0.45	2.26	29	3
1:A:27:PHE:CD2	1:A:44:VAL:HG12	0.45	2.46	8	7
1:A:74:PHE:CE1	1:A:78:LEU:HD21	0.45	2.47	39	3
1:A:20:PHE:CE1	1:A:81:MET:CG	0.45	2.99	16	2
1:A:38:THR:HG23	1:A:71:THR:CA	0.45	2.41	35	1
1:A:6:LYS:O	1:A:9:VAL:HG12	0.45	2.11	33	4
1:A:27:PHE:CE2	1:A:44:VAL:HG13	0.45	2.46	2	1
1:A:41:LEU:CD1	1:A:61:ILE:HD11	0.45	2.34	14	1
1:A:36:ILE:CG1	1:A:72:VAL:HB	0.44	2.43	4	6
1:A:17:LYS:CD	1:A:78:LEU:HD21	0.44	2.43	2	1
1:A:42:GLY:N	1:A:57:LEU:HD22	0.44	2.26	11	1
1:A:7:ALA:O	1:A:11:GLN:HG2	0.44	2.12	36	1
1:A:28:ILE:O	1:A:28:ILE:HD13	0.43	2.12	35	4
1:A:5:TYR:CE1	1:A:83:ARG:HA	0.43	2.48	36	1
1:A:61:ILE:HA	1:A:64:VAL:HG12	0.43	1.90	25	3
1:A:54:PRO:HA	1:A:57:LEU:CD2	0.43	2.43	23	1
1:A:9:VAL:HA	1:A:12:LEU:HG	0.43	1.91	20	1
1:A:44:VAL:HG11	1:A:77:PHE:HE1	0.43	1.73	17	1
1:A:24:PHE:CE1	1:A:36:ILE:HG23	0.43	2.49	28	1
1:A:51:ASN:N	1:A:52:PRO:CD	0.43	2.82	29	1
1:A:21:LYS:HB2	1:A:74:PHE:CZ	0.43	2.48	22	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HD11	1:A:47:MET:HE3	0.43	1.90	24	1
1:A:17:LYS:HD3	1:A:78:LEU:CD2	0.42	2.44	25	1
1:A:74:PHE:CZ	1:A:78:LEU:HD21	0.42	2.49	37	1
1:A:28:ILE:HD12	1:A:31:ALA:CB	0.42	2.45	11	1
1:A:64:VAL:CG2	1:A:79:VAL:HG12	0.42	2.45	29	1
1:A:12:LEU:N	1:A:12:LEU:HD12	0.42	2.30	2	1
1:A:38:THR:HG22	1:A:70:GLY:O	0.42	2.14	3	1
1:A:57:LEU:HD22	1:A:57:LEU:C	0.42	2.35	24	1
1:A:20:PHE:CE2	1:A:48:LEU:HD11	0.42	2.49	14	1
1:A:12:LEU:HD22	1:A:16:GLN:HG2	0.42	1.91	20	1
1:A:39:LYS:CD	1:A:40:GLU:HG2	0.42	2.45	37	1
1:A:8:ALA:HB1	1:A:82:VAL:HG11	0.42	1.91	39	1
1:A:28:ILE:HD12	1:A:28:ILE:C	0.41	2.35	20	2
1:A:23:ALA:O	1:A:27:PHE:CD2	0.41	2.73	38	3
1:A:5:TYR:CE2	1:A:83:ARG:HA	0.41	2.50	20	1
1:A:28:ILE:HG13	1:A:31:ALA:HB3	0.41	1.93	30	1
1:A:41:LEU:O	1:A:44:VAL:HG22	0.41	2.16	8	1
1:A:35:CYS:HB3	1:A:71:THR:HB	0.41	1.92	40	1
1:A:34:GLY:C	1:A:35:CYS:SG	0.41	2.99	7	2
1:A:81:MET:HB3	1:A:81:MET:HE2	0.41	1.71	8	1
1:A:38:THR:HG23	1:A:71:THR:N	0.41	2.30	27	1
1:A:45:MET:SD	1:A:46:ARG:HG3	0.41	2.55	29	1
1:A:44:VAL:CG1	1:A:77:PHE:CZ	0.41	3.04	17	1
1:A:61:ILE:O	1:A:65:ASP:HB2	0.41	2.16	28	1
1:A:8:ALA:HB3	1:A:82:VAL:HG11	0.41	1.93	18	1
1:A:74:PHE:CE1	1:A:78:LEU:CD1	0.41	3.04	40	1
1:A:44:VAL:HG12	1:A:48:LEU:CD1	0.40	2.46	28	1
1:A:6:LYS:HA	1:A:9:VAL:HG12	0.40	1.91	36	1
1:A:20:PHE:CZ	1:A:81:MET:HB2	0.40	2.52	10	1
1:A:28:ILE:CD1	1:A:31:ALA:CB	0.40	2.99	30	1
1:A:53:THR:CB	1:A:54:PRO:CD	0.40	2.99	6	1
1:A:41:LEU:CD1	1:A:44:VAL:HG22	0.40	2.46	22	1
1:A:57:LEU:O	1:A:61:ILE:HG12	0.40	2.16	40	1
1:A:57:LEU:C	1:A:57:LEU:HD12	0.40	2.36	17	2

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	79/89 (89%)	74±1 (94±1%)	5±1 (6±1%)	0±0 (0±1%)	44	80
All	All	3160/3560 (89%)	2958 (94%)	194 (6%)	8 (0%)	44	80

All 2 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	52	PRO	5
1	A	65	ASP	3

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	69/79 (87%)	58±3 (83±4%)	11±3 (17±4%)	5	41
All	All	2760/3160 (87%)	2301 (83%)	459 (17%)	5	41

All 46 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	13	THR	40
1	A	77	PHE	40
1	A	12	LEU	34
1	A	65	ASP	33
1	A	41	LEU	27
1	A	21	LYS	26
1	A	37	SER	23
1	A	6	LYS	19
1	A	16	GLN	18
1	A	25	ASP	16
1	A	39	LYS	16
1	A	44	VAL	15
1	A	45	MET	14
1	A	50	GLN	11

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Mol	Chain	Res	Type	Models (Total)
1	A	47	MET	11
1	A	28	ILE	10
1	A	32	GLU	7
1	A	62	ASP	7
1	A	43	LYS	6
1	A	83	ARG	6
1	A	80	MET	6
1	A	66	GLU	6
1	A	81	MET	5
1	A	30	ASP	5
1	A	46	ARG	5
1	A	57	LEU	5
1	A	15	GLU	5
1	A	67	ASP	4
1	A	59	GLU	4
1	A	17	LYS	4
1	A	14	ASP	3
1	A	10	GLU	3
1	A	56	GLU	3
1	A	48	LEU	3
1	A	36	ILE	2
1	A	73	ASP	2
1	A	33	ASP	2
1	A	63	GLU	2
1	A	40	GLU	2
1	A	24	PHE	2
1	A	79	VAL	2
1	A	60	MET	1
1	A	51	ASN	1
1	A	69	SER	1
1	A	11	GLN	1
1	A	78	LEU	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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