Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 06:16 PM EST

PDB ID	:	2F52
Title	:	Solution structure of cold shock protein CspB from Bacillus subtilis in complex with heptathymidine
Authors	:	Zeeb, M.; Sticht, H.; Balbach, J.
Deposited on	:	2005-11-25

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:

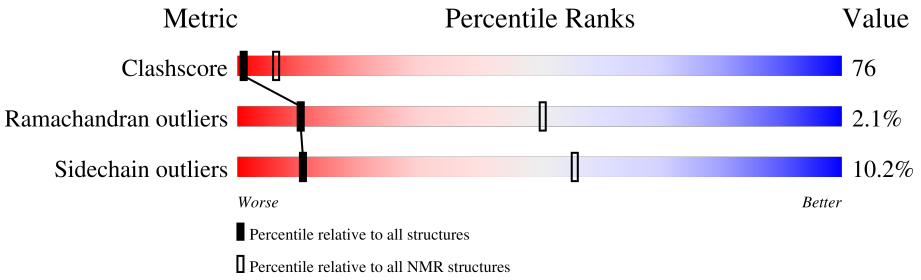
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (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	67	22% 52% 7% 18%

2 Ensemble composition and analysis (i)

This entry contains 18 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *smalest pair-wise rmsd*.

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:2-A:10, A:15-A:33, A:41-A:67 (55)	0.20	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 4 clusters and 6 single-model clusters were found.

Cluster number	Models
1	3, 6, 10, 13, 14
2	4, 8, 17
3	9, 15
4	5, 7
Single-model clusters	1; 2; 11; 12; 16; 18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1014 atoms, of which 493 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cold shock protein cspB.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	67	1014	331	493	85	104	1	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: Cold shock protein cspB

Chain A: 22% 52% 7% 18%

M1 L2 E3 G4 K5 V6 K7 W8 F9 N10 S11 E12 K13 G14 F15 G16 F17 I18 E19 V20 Q23 D24 D25 V26 F27 V28 H29 F30 S31 A32 I33 Q34 G35 E36 G37 F38 K39 T40 L41 E42 Q45 A46 V47 S48 F49 E50 I51 V52 R56 G57 P58 Q59 A60 A61 N62 V63 T64

K65 E66 A67

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: Cold shock protein cspB

Chain A: 24% 54% • 18%

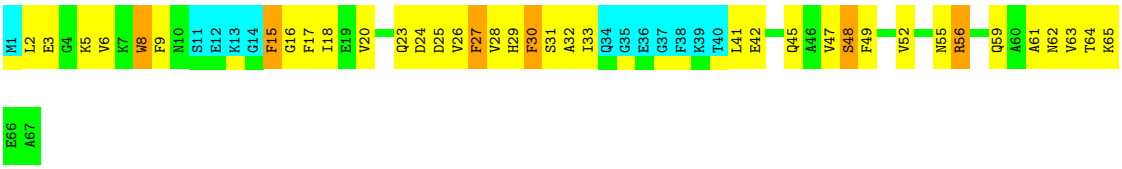
M1 G4 K5 V6 K7 W8 F9 N10 S11 E12 K13 G14 F15 G16 F17 I18 E19 V20 Q23 D24 D25 V26 F27 V28 H29 F30 S31 A32 I33 Q34 G35 E36 G37 F38 K39 T40 L41 E42 E43 G44 Q45 A46 V47 S48 F49 E50 I51 V52 R56 G57 P58 Q59 A60 A61 N62 V63 T64

K65 E66 A67

4.2.2 Score per residue for model 2

• Molecule 1: Cold shock protein cspB

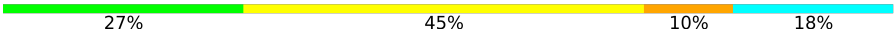
Chain A: 27% 46% 9% 18%

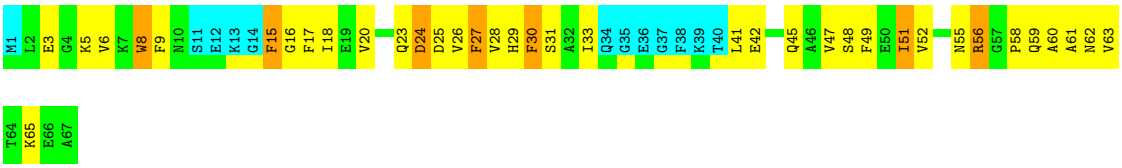


4.2.3 Score per residue for model 3

- Molecule 1: Cold shock protein cspB

Chain A:

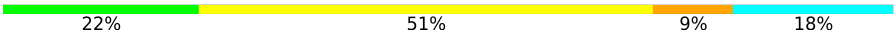


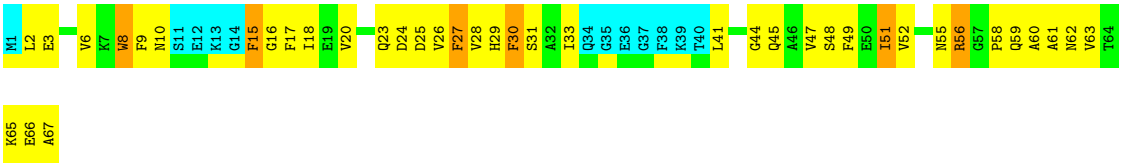


4.2.4 Score per residue for model 4

- Molecule 1: Cold shock protein cspB

Chain A:

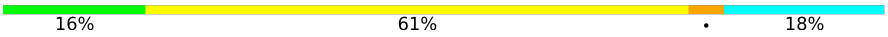


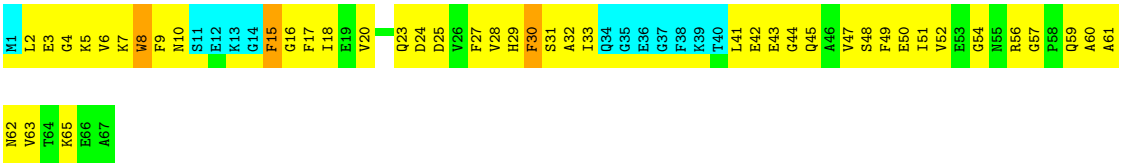


4.2.5 Score per residue for model 5

- Molecule 1: Cold shock protein cspB

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: Cold shock protein cspB

Chain A: 24% 54% • 18%

M1 L2 E3 G4 K5 V6 K7 W8 F9 N10 S11 E12 K13 G14 F15 G16 F17 I18 E19 V20 E21 G22 Q23 D24 D25 V26 F27 V28 H29 F30 S31 A32 I33 Q34 G35 E36 G37 F38 K39 T40 L41 E42 Q45 A46 V47 S48 F49 E50 I51 R56 Q59 A60 A61 N62 V63 T64 K65

E66 A67

4.2.7 Score per residue for model 7

- Molecule 1: Cold shock protein cspB

Chain A: 22% 55% • 18%

M1 L2 E3 G4 K5 V6 K7 W8 F9 N10 S11 E12 K13 G14 F15 G16 F17 I18 E19 V20 Q23 D24 D25 V26 F27 V28 H29 F30 S31 A32 I33 Q34 G35 E36 G37 F38 K39 T40 L41 E42 E43 G44 Q45 A46 V47 S48 F49 E50 I51 V52 R56 Q59 A60 A61 N62 V63 T64

K65 E66 A67

4.2.8 Score per residue for model 8

- Molecule 1: Cold shock protein cspB

Chain A: 28% 49% • 18%

M1 L2 E3 V6 K7 W8 F9 N10 S11 E12 K13 G14 F15 G16 F17 I18 E19 V20 D24 D25 V26 F27 V28 H29 F30 S31 A32 I33 Q34 G35 E36 G37 F38 K39 T40 L41 E42 Q45 A46 V47 S48 F49 E50 I51 V52 R56 G57 P58 Q59 A60 A61 N62 V63 T64 K65 E66

A67

4.2.9 Score per residue for model 9

- Molecule 1: Cold shock protein cspB

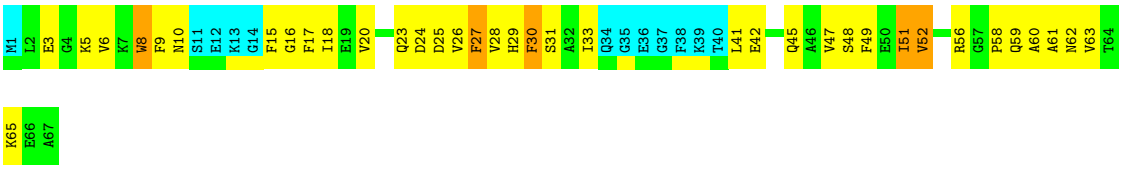
Chain A: 34% 42% 6% 18%

M1 L2 E3 G4 K5 V6 K7 W8 F9 N10 S11 E12 K13 G14 F15 G16 F17 I18 E19 V20 D24 D25 V26 F27 V28 H29 F30 S31 A32 I33 Q34 G35 E36 G37 F38 K39 T40 L41 E42 Q45 A46 V47 S48 F49 V52 R56 Q59 A60 A61 N62 V63 A67

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Cold shock protein cspB

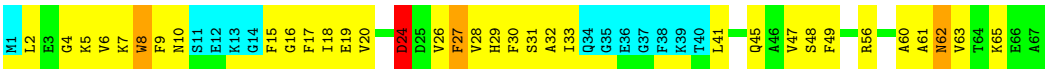
Chain A: 27% 48% 7% 18%



4.2.11 Score per residue for model 11

- Molecule 1: Cold shock protein cspB

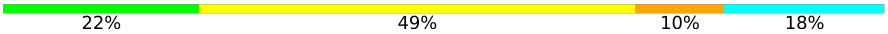
Chain A:

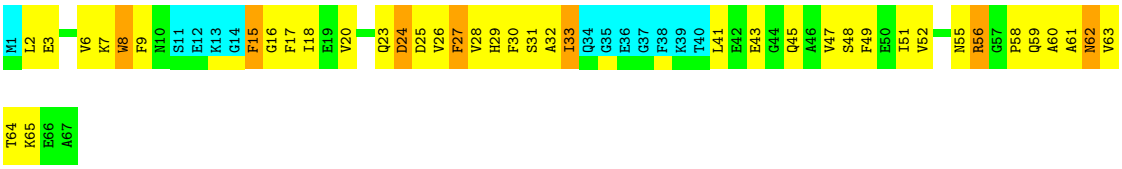


4.2.12 Score per residue for model 12

- Molecule 1: Cold shock protein cspB

Chain A:

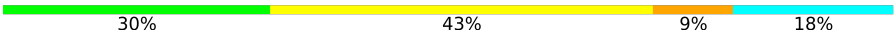


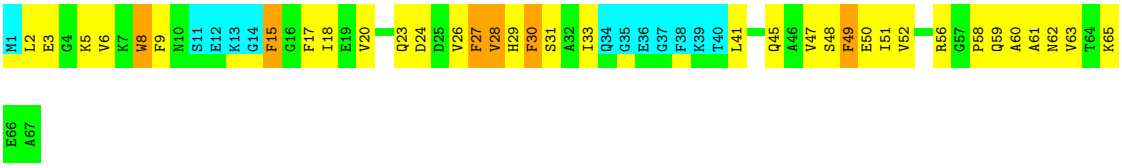


4.2.13 Score per residue for model 13

- Molecule 1: Cold shock protein cspB

Chain A:

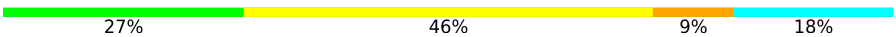




4.2.14 Score per residue for model 14

- Molecule 1: Cold shock protein cspB

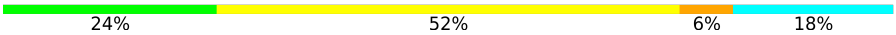
Chain A:

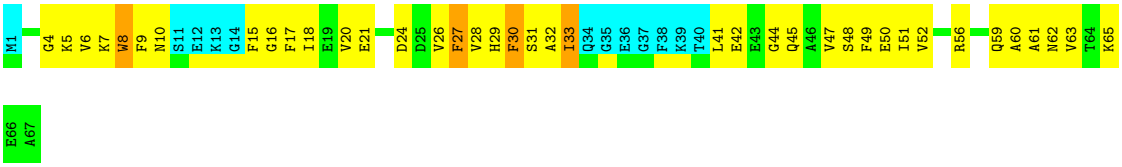


4.2.15 Score per residue for model 15

- Molecule 1: Cold shock protein cspB

Chain A:

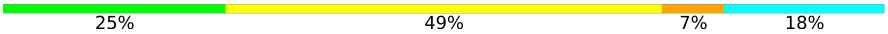


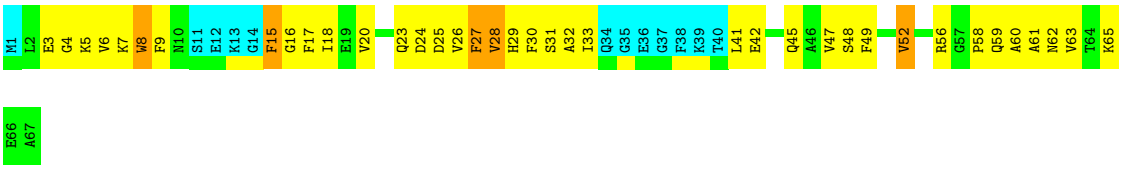


4.2.16 Score per residue for model 16

- Molecule 1: Cold shock protein cspB

Chain A:

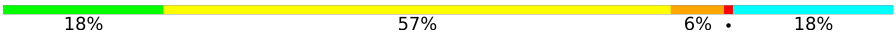


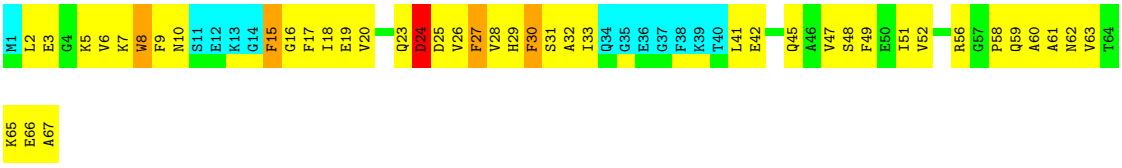


4.2.17 Score per residue for model 17

- Molecule 1: Cold shock protein cspB

Chain A:

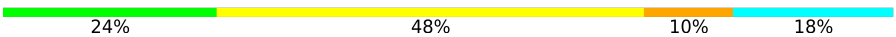


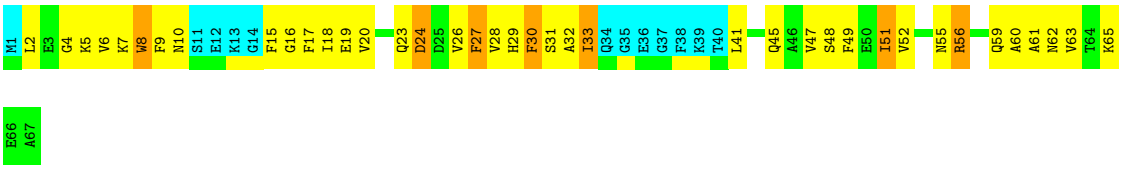


4.2.18 Score per residue for model 18

- Molecule 1: Cold shock protein cspB

Chain A:




M1
L2
E3
G4
K5
V6
K7
W8
F9
N10
S11
E12
K13
G14
F15
G16
F17
I18
E19
V20
Q23
D24
D25
V26
F27
V28
H29
F30
S31
A32
I33
Q34
G35
E36
G37
F38
K39
T40
L41
Q45
A46
V47
S48
F49
E50
I51
V52
N55
R56
Q59
A60
A61
N62
V63
T64
K65

E66
A67

5 Refinement protocol and experimental data overview (i)

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

Of the 120 calculated structures, 18 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	structure solution	1.2.1
X-PLOR	refinement	1.2.1

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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.0
All	All	0	18

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	56	ARG	Sidechain	18

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	432	406	406	64±7
All	All	7776	7308	7308	1144

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 76.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HD12	1:A:28:VAL:HG21	1.06	1.12	12	16
1:A:18:ILE:CD1	1:A:28:VAL:HG21	1.03	1.84	11	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HD12	1:A:28:VAL:CG2	1.02	1.83	9	15
1:A:41:LEU:HD23	1:A:47:VAL:HG11	0.98	1.36	15	6
1:A:33:ILE:HG23	1:A:63:VAL:HG12	0.96	1.37	12	8
1:A:33:ILE:HD11	1:A:41:LEU:HD11	0.95	1.33	16	8
1:A:33:ILE:HD13	1:A:41:LEU:HD13	0.93	1.39	1	4
1:A:33:ILE:HD13	1:A:41:LEU:CD1	0.91	1.95	1	7
1:A:33:ILE:HD11	1:A:41:LEU:CD1	0.89	1.97	11	3
1:A:41:LEU:HD21	1:A:63:VAL:HG11	0.86	1.47	15	7
1:A:33:ILE:CD1	1:A:41:LEU:HD11	0.84	2.02	3	12
1:A:33:ILE:HG23	1:A:63:VAL:CG1	0.82	2.03	12	3
1:A:33:ILE:HG21	1:A:65:LYS:NZ	0.82	1.88	13	5
1:A:2:LEU:HD12	1:A:2:LEU:N	0.81	1.91	5	9
1:A:6:VAL:HG23	1:A:45:GLN:O	0.80	1.76	12	18
1:A:47:VAL:HG12	1:A:65:LYS:HA	0.80	1.52	14	7
1:A:18:ILE:HD11	1:A:41:LEU:HD22	0.79	1.55	6	4
1:A:18:ILE:HD13	1:A:47:VAL:HG21	0.78	1.56	9	10
1:A:30:PHE:CD1	1:A:31:SER:N	0.77	2.53	16	18
1:A:28:VAL:CG1	1:A:63:VAL:HG21	0.77	2.08	11	14
1:A:18:ILE:CD1	1:A:47:VAL:HG21	0.75	2.12	13	14
1:A:33:ILE:HG12	1:A:63:VAL:HG11	0.74	1.59	1	10
1:A:23:GLN:OE1	1:A:51:ILE:HD12	0.74	1.82	14	10
1:A:30:PHE:CG	1:A:31:SER:N	0.71	2.58	12	18
1:A:27:PHE:CG	1:A:27:PHE:O	0.71	2.44	16	1
1:A:29:HIS:CE1	1:A:30:PHE:CD2	0.70	2.79	13	18
1:A:33:ILE:HG21	1:A:41:LEU:HD11	0.70	1.62	1	2
1:A:52:VAL:CG1	1:A:61:ALA:HB2	0.70	2.16	1	2
1:A:28:VAL:HG22	1:A:60:ALA:CB	0.70	2.16	18	13
1:A:29:HIS:CE1	1:A:30:PHE:CE2	0.69	2.80	16	18
1:A:33:ILE:CG1	1:A:63:VAL:HG11	0.69	2.17	4	12
1:A:8:TRP:CE3	1:A:17:PHE:CD2	0.69	2.81	5	14
1:A:3:GLU:O	1:A:20:VAL:HG13	0.69	1.86	4	13
1:A:8:TRP:CZ3	1:A:17:PHE:CD2	0.68	2.82	13	14
1:A:41:LEU:CD2	1:A:47:VAL:HG11	0.68	2.17	15	1
1:A:33:ILE:CG1	1:A:41:LEU:HD11	0.68	2.18	17	13
1:A:8:TRP:CD2	1:A:9:PHE:N	0.67	2.63	11	13
1:A:41:LEU:HD21	1:A:63:VAL:CG1	0.67	2.18	15	4
1:A:33:ILE:HG21	1:A:65:LYS:HZ2	0.66	1.49	10	3
1:A:33:ILE:HG21	1:A:65:LYS:HZ1	0.66	1.49	4	3
1:A:41:LEU:N	1:A:41:LEU:HD12	0.65	2.06	9	12
1:A:8:TRP:CG	1:A:9:PHE:N	0.65	2.65	18	18
1:A:9:PHE:CD2	1:A:41:LEU:O	0.65	2.50	15	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:PHE:CD1	1:A:15:PHE:N	0.62	2.68	11	12
1:A:2:LEU:N	1:A:2:LEU:CD1	0.62	2.62	8	9
1:A:33:ILE:HG12	1:A:41:LEU:HD11	0.62	1.70	15	9
1:A:18:ILE:HD13	1:A:47:VAL:CG2	0.62	2.24	13	14
1:A:52:VAL:HG23	1:A:59:GLN:HB2	0.62	1.70	9	4
1:A:8:TRP:O	1:A:8:TRP:CE3	0.61	2.53	12	9
1:A:33:ILE:CD1	1:A:41:LEU:CD1	0.60	2.78	1	8
1:A:28:VAL:HG13	1:A:63:VAL:HG21	0.60	1.72	11	14
1:A:28:VAL:HG22	1:A:60:ALA:HB2	0.60	1.73	14	3
1:A:18:ILE:HD11	1:A:47:VAL:HG21	0.60	1.74	16	4
1:A:33:ILE:CG1	1:A:63:VAL:CG1	0.59	2.80	5	9
1:A:41:LEU:CD1	1:A:41:LEU:N	0.59	2.65	4	8
1:A:52:VAL:HG13	1:A:61:ALA:HB2	0.59	1.72	1	1
1:A:27:PHE:CD1	1:A:28:VAL:N	0.59	2.70	10	5
1:A:8:TRP:CD2	1:A:8:TRP:C	0.58	2.77	12	18
1:A:18:ILE:CD1	1:A:47:VAL:CG2	0.58	2.81	1	4
1:A:30:PHE:O	1:A:33:ILE:HD12	0.58	1.97	11	1
1:A:8:TRP:CE3	1:A:8:TRP:O	0.58	2.56	13	5
1:A:26:VAL:HG13	1:A:59:GLN:C	0.58	2.19	7	5
1:A:33:ILE:HD13	1:A:41:LEU:HD11	0.57	1.76	14	6
1:A:18:ILE:HD11	1:A:41:LEU:CD2	0.57	2.29	2	2
1:A:27:PHE:CE1	1:A:28:VAL:O	0.57	2.57	12	3
1:A:29:HIS:O	1:A:33:ILE:CD1	0.57	2.52	12	2
1:A:5:LYS:C	1:A:18:ILE:HG23	0.57	2.20	11	6
1:A:29:HIS:NE2	1:A:30:PHE:CD2	0.57	2.72	16	1
1:A:33:ILE:HD11	1:A:41:LEU:HD21	0.57	1.75	14	1
1:A:8:TRP:CZ3	1:A:16:GLY:HA2	0.56	2.35	9	17
1:A:5:LYS:O	1:A:18:ILE:HG23	0.56	1.99	17	8
1:A:29:HIS:O	1:A:33:ILE:HD12	0.56	2.00	12	4
1:A:27:PHE:O	1:A:60:ALA:N	0.56	2.39	12	8
1:A:10:ASN:HB3	1:A:15:PHE:CE1	0.56	2.35	1	3
1:A:30:PHE:CD1	1:A:30:PHE:C	0.56	2.79	9	18
1:A:33:ILE:HG21	1:A:65:LYS:HE2	0.56	1.76	14	2
1:A:48:SER:O	1:A:63:VAL:HA	0.56	2.01	1	15
1:A:27:PHE:CG	1:A:28:VAL:N	0.55	2.74	8	10
1:A:32:ALA:O	1:A:63:VAL:HB	0.55	2.01	15	5
1:A:5:LYS:N	1:A:18:ILE:HG23	0.55	2.16	11	5
1:A:33:ILE:HD12	1:A:33:ILE:N	0.55	2.17	9	2
1:A:28:VAL:HG11	1:A:63:VAL:HG21	0.55	1.77	11	3
1:A:33:ILE:HG12	1:A:63:VAL:CG1	0.55	2.31	13	4
1:A:9:PHE:CG	1:A:41:LEU:O	0.54	2.60	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HG13	1:A:63:VAL:CG1	0.54	2.33	11	11
1:A:27:PHE:C	1:A:27:PHE:CD1	0.54	2.81	7	3
1:A:49:PHE:HB2	1:A:61:ALA:O	0.54	2.01	15	17
1:A:8:TRP:O	1:A:16:GLY:HA3	0.54	2.03	11	2
1:A:23:GLN:OE1	1:A:51:ILE:CD1	0.54	2.56	6	7
1:A:61:ALA:O	1:A:62:ASN:C	0.54	2.46	14	18
1:A:24:ASP:OD1	1:A:24:ASP:N	0.53	2.41	11	1
1:A:8:TRP:CZ2	1:A:10:ASN:HB2	0.53	2.39	11	11
1:A:20:VAL:HG21	1:A:26:VAL:HG21	0.53	1.80	17	15
1:A:7:LYS:N	1:A:17:PHE:O	0.52	2.40	18	3
1:A:52:VAL:CG2	1:A:59:GLN:HB2	0.52	2.35	14	16
1:A:33:ILE:HG23	1:A:63:VAL:O	0.52	2.04	11	1
1:A:8:TRP:O	1:A:16:GLY:CA	0.52	2.57	1	3
1:A:41:LEU:HD12	1:A:41:LEU:H	0.52	1.62	9	3
1:A:29:HIS:O	1:A:32:ALA:N	0.52	2.40	11	7
1:A:8:TRP:CE3	1:A:8:TRP:C	0.52	2.83	4	11
1:A:25:ASP:N	1:A:25:ASP:OD1	0.52	2.42	8	9
1:A:49:PHE:CD1	1:A:49:PHE:C	0.52	2.83	7	16
1:A:4:GLY:C	1:A:18:ILE:CG2	0.52	2.78	11	5
1:A:6:VAL:O	1:A:44:GLY:N	0.51	2.42	7	4
1:A:28:VAL:CG2	1:A:63:VAL:HG21	0.51	2.35	16	1
1:A:26:VAL:HG21	1:A:51:ILE:HD11	0.51	1.82	12	3
1:A:8:TRP:C	1:A:8:TRP:CE3	0.51	2.85	14	5
1:A:23:GLN:O	1:A:24:ASP:O	0.51	2.29	17	6
1:A:27:PHE:CD1	1:A:27:PHE:C	0.50	2.82	13	4
1:A:15:PHE:HB3	1:A:29:HIS:HA	0.50	1.83	13	8
1:A:28:VAL:CG2	1:A:33:ILE:HD11	0.50	2.35	13	1
1:A:55:ASN:CG	1:A:56:ARG:N	0.50	2.65	2	3
1:A:6:VAL:HB	1:A:42:GLU:O	0.49	2.08	2	8
1:A:48:SER:O	1:A:49:PHE:HB3	0.49	2.08	13	18
1:A:29:HIS:O	1:A:32:ALA:HB3	0.49	2.07	16	5
1:A:28:VAL:HG12	1:A:33:ILE:HD11	0.49	1.83	9	4
1:A:52:VAL:O	1:A:58:PRO:HA	0.49	2.07	10	6
1:A:26:VAL:HG12	1:A:60:ALA:HB2	0.49	1.85	8	2
1:A:15:PHE:HB2	1:A:28:VAL:O	0.48	2.07	9	13
1:A:27:PHE:CE2	1:A:59:GLN:HB3	0.48	2.43	18	2
1:A:25:ASP:O	1:A:58:PRO:HG2	0.48	2.07	12	4
1:A:33:ILE:CD1	1:A:41:LEU:HD21	0.48	2.39	14	1
1:A:6:VAL:CB	1:A:42:GLU:O	0.48	2.62	2	7
1:A:5:LYS:NZ	1:A:21:GLU:OE2	0.48	2.47	15	1
1:A:7:LYS:O	1:A:43:GLU:OE2	0.47	2.32	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:VAL:HG11	1:A:23:GLN:OE1	0.47	2.09	16	2
1:A:47:VAL:HG23	1:A:49:PHE:CE2	0.47	2.44	5	7
1:A:18:ILE:CD1	1:A:28:VAL:HG11	0.47	2.39	16	2
1:A:47:VAL:HA	1:A:64:THR:O	0.47	2.09	12	3
1:A:41:LEU:HD12	1:A:65:LYS:HE3	0.47	1.86	13	2
1:A:41:LEU:H	1:A:41:LEU:HD12	0.47	1.68	6	1
1:A:47:VAL:HG23	1:A:49:PHE:CD2	0.47	2.44	15	4
1:A:6:VAL:HA	1:A:18:ILE:HG12	0.47	1.86	11	3
1:A:33:ILE:CD1	1:A:41:LEU:HD13	0.47	2.26	1	1
1:A:28:VAL:HG11	1:A:41:LEU:HD21	0.47	1.86	2	2
1:A:52:VAL:HG11	1:A:61:ALA:HB2	0.47	1.87	1	1
1:A:28:VAL:HG22	1:A:60:ALA:HB3	0.47	1.86	15	1
1:A:18:ILE:CG2	1:A:19:GLU:N	0.47	2.77	1	3
1:A:7:LYS:CG	1:A:8:TRP:N	0.47	2.78	17	2
1:A:20:VAL:HG21	1:A:26:VAL:CG2	0.46	2.41	8	9
1:A:8:TRP:CZ2	1:A:10:ASN:CB	0.46	2.98	5	1
1:A:20:VAL:CG2	1:A:26:VAL:CG2	0.46	2.94	10	4
1:A:27:PHE:CD1	1:A:59:GLN:HB3	0.46	2.45	15	1
1:A:66:GLU:O	1:A:67:ALA:O	0.46	2.34	17	2
1:A:6:VAL:CG1	1:A:43:GLU:HA	0.46	2.41	5	2
1:A:33:ILE:HG12	1:A:41:LEU:HD21	0.46	1.86	12	1
1:A:8:TRP:CH2	1:A:10:ASN:HB2	0.46	2.46	18	3
1:A:52:VAL:O	1:A:52:VAL:HG23	0.45	2.10	14	8
1:A:29:HIS:O	1:A:32:ALA:CB	0.45	2.65	11	1
1:A:33:ILE:HG13	1:A:63:VAL:HG11	0.45	1.88	14	3
1:A:41:LEU:HD12	1:A:41:LEU:N	0.45	2.26	6	1
1:A:28:VAL:HB	1:A:60:ALA:CB	0.45	2.42	13	2
1:A:42:GLU:O	1:A:43:GLU:C	0.45	2.54	1	1
1:A:5:LYS:O	1:A:18:ILE:HA	0.45	2.11	11	1
1:A:4:GLY:HA3	1:A:18:ILE:CG2	0.45	2.42	1	4
1:A:28:VAL:HB	1:A:60:ALA:HB3	0.45	1.88	16	2
1:A:29:HIS:O	1:A:30:PHE:C	0.45	2.54	18	10
1:A:5:LYS:N	1:A:18:ILE:CG2	0.45	2.80	11	1
1:A:19:GLU:OE1	1:A:25:ASP:OD1	0.45	2.34	17	1
1:A:9:PHE:O	1:A:9:PHE:CG	0.44	2.70	5	1
1:A:27:PHE:CE1	1:A:59:GLN:HB3	0.44	2.48	15	2
1:A:9:PHE:HB2	1:A:15:PHE:O	0.44	2.12	11	1
1:A:48:SER:O	1:A:49:PHE:CB	0.44	2.65	13	4
1:A:18:ILE:HG22	1:A:19:GLU:N	0.44	2.28	18	1
1:A:47:VAL:CA	1:A:64:THR:O	0.44	2.65	12	1
1:A:9:PHE:HA	1:A:15:PHE:O	0.44	2.13	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:PHE:CB	1:A:61:ALA:O	0.44	2.66	15	2
1:A:27:PHE:CZ	1:A:29:HIS:HB2	0.44	2.47	7	11
1:A:9:PHE:HA	1:A:16:GLY:HA2	0.44	1.90	18	2
1:A:32:ALA:O	1:A:63:VAL:N	0.44	2.44	16	1
1:A:28:VAL:HG11	1:A:41:LEU:CD2	0.44	2.43	18	1
1:A:27:PHE:O	1:A:27:PHE:CD1	0.44	2.71	16	1
1:A:52:VAL:O	1:A:59:GLN:N	0.43	2.51	4	1
1:A:26:VAL:CG1	1:A:60:ALA:N	0.43	2.81	7	1
1:A:28:VAL:HA	1:A:60:ALA:HB3	0.43	1.90	16	1
1:A:55:ASN:O	1:A:56:ARG:C	0.43	2.54	18	2
1:A:52:VAL:HG23	1:A:59:GLN:CB	0.43	2.43	10	1
1:A:9:PHE:CA	1:A:15:PHE:O	0.43	2.66	11	1
1:A:10:ASN:N	1:A:15:PHE:O	0.43	2.45	1	1
1:A:7:LYS:HG3	1:A:8:TRP:N	0.43	2.29	17	2
1:A:49:PHE:HB3	1:A:63:VAL:HA	0.43	1.89	12	4
1:A:8:TRP:CE3	1:A:16:GLY:HA2	0.43	2.48	18	3
1:A:26:VAL:CG2	1:A:51:ILE:HG12	0.43	2.43	7	1
1:A:9:PHE:HA	1:A:16:GLY:CA	0.42	2.43	1	1
1:A:33:ILE:CG2	1:A:41:LEU:HD11	0.42	2.41	1	1
1:A:41:LEU:HD12	1:A:65:LYS:HZ1	0.42	1.73	12	1
1:A:5:LYS:NZ	1:A:21:GLU:CD	0.42	2.73	15	1
1:A:49:PHE:HA	1:A:62:ASN:O	0.42	2.15	11	2
1:A:28:VAL:HG21	1:A:41:LEU:HD21	0.42	1.91	13	1
1:A:66:GLU:O	1:A:67:ALA:HB3	0.42	2.14	17	1
1:A:50:GLU:HA	1:A:50:GLU:OE1	0.42	2.15	13	1
1:A:6:VAL:HG12	1:A:43:GLU:HA	0.42	1.91	5	1
1:A:26:VAL:HG21	1:A:51:ILE:CG1	0.42	2.44	6	1
1:A:7:LYS:NZ	1:A:17:PHE:HB3	0.41	2.30	7	1
1:A:33:ILE:HG21	1:A:65:LYS:CE	0.41	2.45	14	1
1:A:2:LEU:HD13	1:A:50:GLU:HA	0.41	1.92	5	1
1:A:41:LEU:CD1	1:A:65:LYS:NZ	0.41	2.82	5	1
1:A:54:GLY:N	1:A:57:GLY:O	0.41	2.54	5	1
1:A:50:GLU:OE1	1:A:50:GLU:HA	0.41	2.15	15	1
1:A:21:GLU:OE1	1:A:21:GLU:HA	0.41	2.15	6	1
1:A:15:PHE:CB	1:A:29:HIS:HA	0.41	2.45	7	1
1:A:27:PHE:CD1	1:A:59:GLN:HG2	0.41	2.50	7	1
1:A:41:LEU:HD12	1:A:65:LYS:CE	0.41	2.45	13	1
1:A:9:PHE:CE2	1:A:41:LEU:O	0.41	2.74	14	1
1:A:26:VAL:HG21	1:A:51:ILE:CD1	0.41	2.45	6	1
1:A:2:LEU:HB2	1:A:49:PHE:O	0.41	2.16	8	3
1:A:2:LEU:CD1	1:A:51:ILE:HD13	0.41	2.45	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:PHE:CE1	1:A:27:PHE:CD1	0.41	3.09	13	1
1:A:33:ILE:HA	1:A:63:VAL:O	0.41	2.15	16	1
1:A:15:PHE:HB2	1:A:29:HIS:HA	0.41	1.92	18	1
1:A:27:PHE:CE1	1:A:29:HIS:HB2	0.41	2.51	18	1
1:A:5:LYS:O	1:A:19:GLU:N	0.40	2.47	11	1
1:A:41:LEU:HD12	1:A:65:LYS:NZ	0.40	2.32	5	1
1:A:2:LEU:HD12	1:A:51:ILE:HD13	0.40	1.93	12	1
1:A:33:ILE:HG12	1:A:41:LEU:CD1	0.40	2.46	9	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	54/67 (81%)	50±1 (93±1%)	2±1 (5±1%)	1±0 (2±1%)	10	50
All	All	972/1206 (81%)	908 (93%)	44 (5%)	20 (2%)	10	50

All 3 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	24	ASP	18
1	A	62	ASN	1
1	A	49	PHE	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	44/53 (83%)	40±1 (90±2%)	4±1 (10±2%)	11	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	792/954 (83%)	711 (90%)	81 (10%)	11 56

All 12 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	8	TRP	18
1	A	27	PHE	18
1	A	30	PHE	14
1	A	15	PHE	9
1	A	51	ILE	7
1	A	7	LYS	3
1	A	52	VAL	3
1	A	33	ILE	3
1	A	24	ASP	2
1	A	28	VAL	2
1	A	48	SER	1
1	A	62	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 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