Full wwPDB NMR Structure Validation Report (i)

Feb 20, 2022 – 01:09 AM EST

PDB ID	:	1U2U
Title	:	Nmr solution structure of a designed heterodimeric leucine zipper
Authors	:	Marti, D.N.; Bosshard, H.R.
Deposited on	:	2004-07-20

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 (1)) were used in the production of this report:

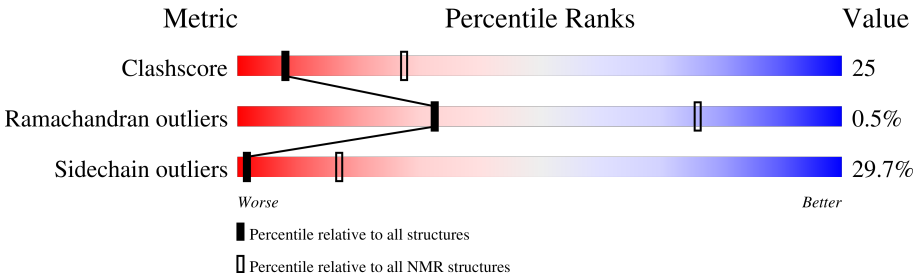
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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	32	38% 34% 28%
2	B	32	19% 53% 6% 22%

2 Ensemble composition and analysis (i)

This entry contains 27 models. Model 27 is the overall representative, medoid model (most similar to other models). The authors have identified model 25 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:27, B:3-B:27 (48)	0.45	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 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 4, 7, 17, 21, 22, 25, 26, 27
2	2, 3, 5, 12, 13, 14, 20
3	10, 11, 18, 23
4	9, 16, 19
Single-model clusters	6; 8; 15; 24

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1003 atoms, of which 509 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called General control protein GCN4.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	32	474	150	228	40	56	1

- Molecule 2 is a protein called General control protein GCN4.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	32	529	156	281	53	39	1

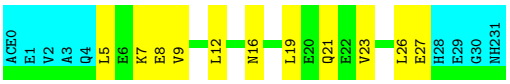
4 Residue-property plots (i)

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: General control protein GCN4

Chain A: 38% 34% 28%



• Molecule 2: General control protein GCN4

Chain B: 19% 53% 6% 22%

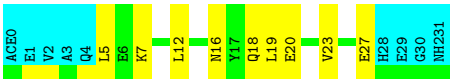
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

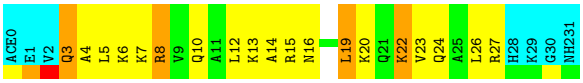
• Molecule 1: General control protein GCN4

Chain A: 44% 28% 28%



• Molecule 2: General control protein GCN4

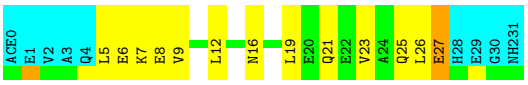
Chain B: 19% 47% 12% 22%



4.2.2 Score per residue for model 2

- Molecule 1: General control protein GCN4

Chain A: 31% 38% • 28%



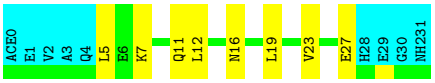
- Molecule 2: General control protein GCN4

Chain B: 31% 34% 12% 22%

4.2.3 Score per residue for model 3

- Molecule 1: General control protein GCN4

Chain A: 47% 25% 28%



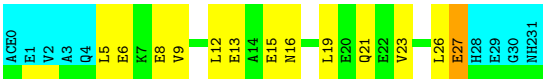
- Molecule 2: General control protein GCN4

Chain B: 25% 41% 12% 22%

4.2.4 Score per residue for model 4

- Molecule 1: General control protein GCN4

Chain A: 31% 38% • 28%



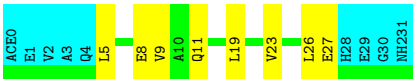
- Molecule 2: General control protein GCN4

Chain B: 25% 44% 9% 22%

4.2.5 Score per residue for model 5

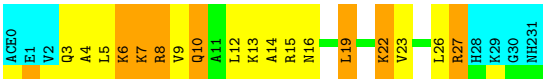
• Molecule 1: General control protein GCN4

Chain A: 47% 25% 28%



• Molecule 2: General control protein GCN4

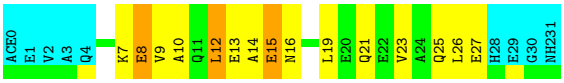
Chain B: 22% 34% 22% 22%



4.2.6 Score per residue for model 6

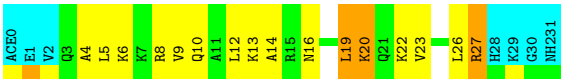
• Molecule 1: General control protein GCN4

Chain A: 25% 38% 9% 28%



• Molecule 2: General control protein GCN4

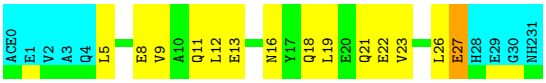
Chain B: 28% 41% 9% 22%



4.2.7 Score per residue for model 7

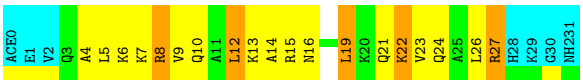
• Molecule 1: General control protein GCN4

Chain A: 28% 41% • 28%



• Molecule 2: General control protein GCN4

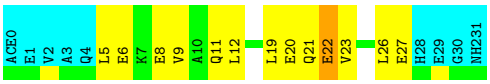
Chain B: 19% 44% 16% 22%



4.2.8 Score per residue for model 8

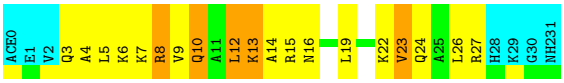
- Molecule 1: General control protein GCN4

Chain A: 31% 38% • 28%



- Molecule 2: General control protein GCN4

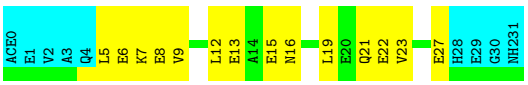
Chain B: 19% 44% 16% 22%



4.2.9 Score per residue for model 9

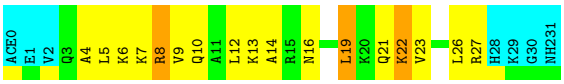
- Molecule 1: General control protein GCN4

Chain A: 28% 44% 28%



- Molecule 2: General control protein GCN4

Chain B: 25% 44% 9% 22%



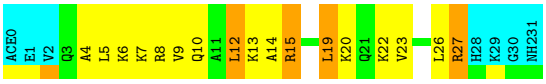
4.2.10 Score per residue for model 10

- Molecule 1: General control protein GCN4

Chain A: 28% 44% 28%

• Molecule 2: General control protein GCN4

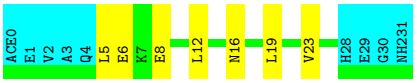
Chain B: 25% 41% 12% 22%



4.2.11 Score per residue for model 11

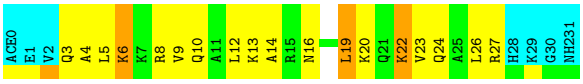
• Molecule 1: General control protein GCN4

Chain A: 50% 22% 28%



• Molecule 2: General control protein GCN4

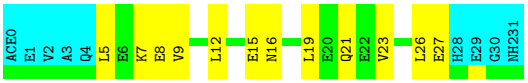
Chain B: 22% 47% 9% 22%



4.2.12 Score per residue for model 12

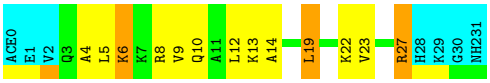
• Molecule 1: General control protein GCN4

Chain A: 34% 38% 28%



• Molecule 2: General control protein GCN4

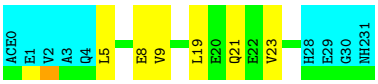
Chain B: 38% 31% 9% 22%



4.2.13 Score per residue for model 13

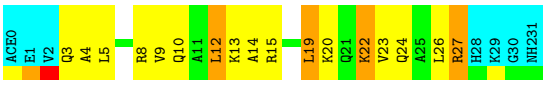
• Molecule 1: General control protein GCN4

Chain A: 53% 19% 28%



• Molecule 2: General control protein GCN4

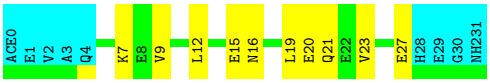
Chain B:



4.2.14 Score per residue for model 14

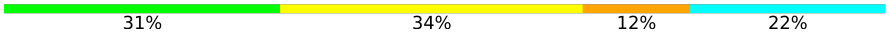
• Molecule 1: General control protein GCN4

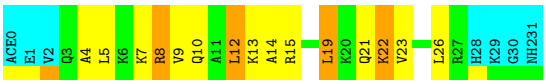
Chain A:



• Molecule 2: General control protein GCN4

Chain B:

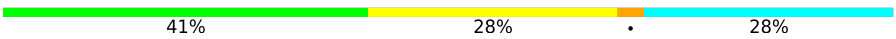




4.2.15 Score per residue for model 15

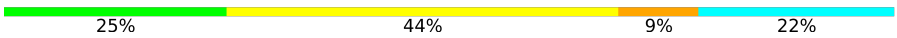
• Molecule 1: General control protein GCN4

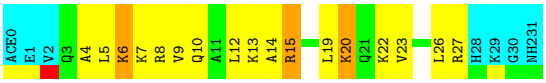
Chain A:



• Molecule 2: General control protein GCN4

Chain B:

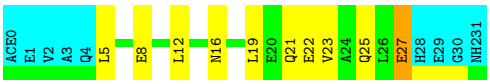




4.2.16 Score per residue for model 16

• Molecule 1: General control protein GCN4

Chain A: 41% 28% • 28%



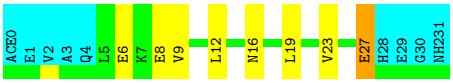
• Molecule 2: General control protein GCN4

Chain B: 25% 44% 9% 22%

4.2.17 Score per residue for model 17

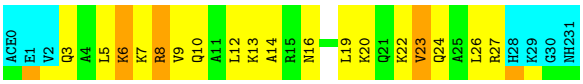
• Molecule 1: General control protein GCN4

Chain A: 47% 22% • 28%



• Molecule 2: General control protein GCN4

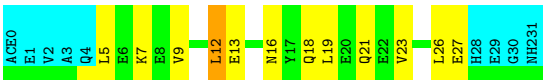
Chain B: 22% 47% 9% 22%



4.2.18 Score per residue for model 18

• Molecule 1: General control protein GCN4

Chain A: 34% 34% • 28%



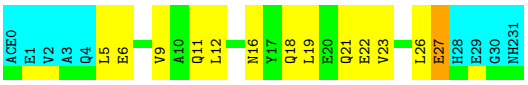
• Molecule 2: General control protein GCN4

Chain B: 25% 44% 9% 22%

4.2.19 Score per residue for model 19

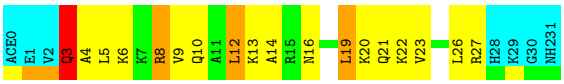
- Molecule 1: General control protein GCN4

Chain A: 31% 38% • 28%



- Molecule 2: General control protein GCN4

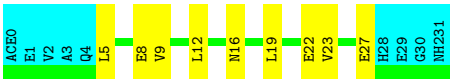
Chain B: 22% 44% 9% • 22%



4.2.20 Score per residue for model 20

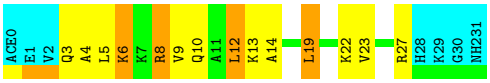
- Molecule 1: General control protein GCN4

Chain A: 44% 28% 28%



- Molecule 2: General control protein GCN4

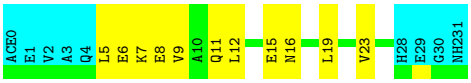
Chain B: 34% 31% 12% 22%



4.2.21 Score per residue for model 21

- Molecule 1: General control protein GCN4

Chain A: 38% 34% 28%



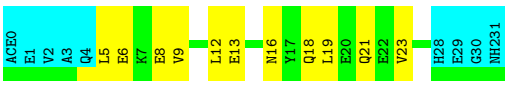
- Molecule 2: General control protein GCN4

Chain B: 22% 47% 9% 22%

4.2.22 Score per residue for model 22

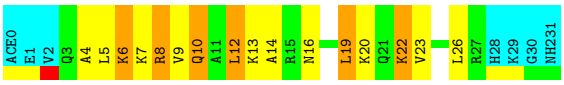
- Molecule 1: General control protein GCN4

Chain A: 38% 34% 28%



- Molecule 2: General control protein GCN4

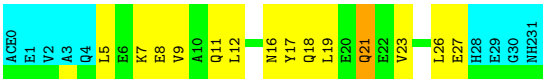
Chain B: 28% 31% 19% 22%



4.2.23 Score per residue for model 23

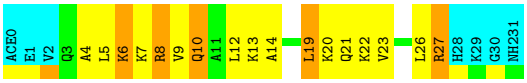
- Molecule 1: General control protein GCN4

Chain A: 28% 41% • 28%



- Molecule 2: General control protein GCN4

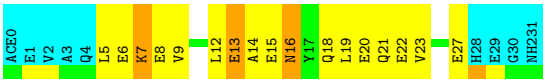
Chain B: 25% 38% 16% 22%



4.2.24 Score per residue for model 24

- Molecule 1: General control protein GCN4

Chain A: 19% 44% 9% 28%



- Molecule 2: General control protein GCN4

Chain B: 22% 41% 16% 22%

ACE0 E1 V2 Q3 A4 L5 K6 K7 R8 V9 Q10 A11 L12 K13 A14 R15 N16 L19 K20 Q21 K22 V23 L26 R27 H28 K29 G30 NH231

4.2.25 Score per residue for model 25

- Molecule 1: General control protein GCN4

Chain A: 34% 38% 28%

ACE0 E1 V2 A3 Q4 L5 E8 Q11 L12 N16 L19 E20 Q21 E22 V23 A24 Q25 L26 E27 H28 E29 G30 NH231

- Molecule 2: General control protein GCN4

Chain B: 31% 38% 9% 22%

ACE0 E1 V2 L5 K6 K7 R8 V9 Q10 A11 L12 K13 A14 R15 L19 K20 Q21 K22 V23 L26 R27 H28 K29 G30 NH231

4.2.26 Score per residue for model 26

- Molecule 1: General control protein GCN4

Chain A: 41% 31% 28%

ACE0 E1 V2 A3 Q4 L5 E8 V9 E15 Q18 L19 E20 Q21 E22 V23 L26 E27 H28 E29 G30 NH231

- Molecule 2: General control protein GCN4

Chain B: 28% 41% 9% 22%

ACE0 E1 V2 Q3 A4 L5 K6 K7 R8 V9 Q10 A11 L12 K13 A14 R15 N16 L19 K22 V23 L26 R27 H28 K29 G30 NH231

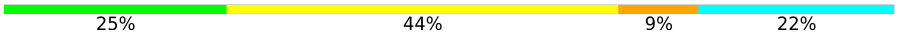
4.2.27 Score per residue for model 27 (medoid)

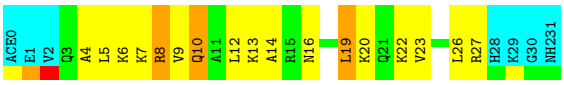
- Molecule 1: General control protein GCN4

Chain A: 38% 34% 28%

ACE0 E1 V2 A3 Q4 L5 E8 V9 L12 N16 Y17 Q18 L19 E20 Q21 E22 V23 E27 H28 E29 G30 NH231

• Molecule 2: General control protein GCN4

Chain B: 



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY/ REGULARIZATION, SIMULATED ANNEALING, MOLECULAR DYNAMICS SIMULATION IN VACUO.*

Of the 50 calculated structures, 27 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, low deviation of experimental pKa values from pKa derived by continuum electrostatics calculations on structures.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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: ACE, NH2

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	189	179	179	14±6
2	B	205	238	238	17±6
All	All	10638	11259	11259	550

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD11	2:B:9:VAL:HG13	1.04	1.26	18	2
1:A:12:LEU:HD12	2:B:12:LEU:HD12	0.86	1.44	6	3
2:B:19:LEU:O	2:B:23:VAL:HG23	0.85	1.72	15	27
1:A:23:VAL:HG13	2:B:26:LEU:HD13	0.84	1.47	24	2
1:A:12:LEU:CD1	2:B:9:VAL:HG13	0.81	2.04	18	2
1:A:9:VAL:HG21	2:B:8:ARG:NE	0.80	1.92	19	1
1:A:19:LEU:O	1:A:23:VAL:HG23	0.80	1.76	8	27
1:A:19:LEU:HD12	2:B:16:ASN:OD1	0.80	1.77	11	17
1:A:23:VAL:HG13	2:B:26:LEU:CD1	0.77	2.09	2	19
2:B:5:LEU:O	2:B:9:VAL:HG23	0.77	1.80	4	9
1:A:12:LEU:HD11	2:B:9:VAL:CG1	0.76	2.10	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:VAL:CG2	2:B:9:VAL:HG22	0.72	2.14	4	13
2:B:19:LEU:C	2:B:23:VAL:HG23	0.72	2.05	5	17
1:A:5:LEU:HD13	2:B:6:LYS:N	0.71	2.01	19	3
1:A:12:LEU:HD22	2:B:13:LYS:HD3	0.71	1.62	6	2
2:B:5:LEU:HD23	2:B:8:ARG:HD3	0.71	1.60	7	2
2:B:10:GLN:O	2:B:14:ALA:HB2	0.71	1.86	18	22
1:A:23:VAL:HG21	2:B:19:LEU:HB3	0.71	1.63	6	15
1:A:12:LEU:HD22	2:B:13:LYS:CD	0.71	2.16	6	2
2:B:15:ARG:CD	2:B:19:LEU:HD11	0.71	2.16	18	2
1:A:6:GLU:HG2	2:B:5:LEU:HD13	0.69	1.62	17	5
1:A:23:VAL:HA	1:A:26:LEU:HD12	0.69	1.65	8	5
1:A:27:GLU:HA	2:B:26:LEU:HD22	0.68	1.65	9	2
1:A:5:LEU:HD22	2:B:6:LYS:CD	0.68	2.19	5	2
2:B:15:ARG:HD3	2:B:19:LEU:HD11	0.66	1.68	18	2
1:A:9:VAL:HG12	1:A:13:GLU:CD	0.66	2.11	24	3
1:A:9:VAL:HG22	2:B:9:VAL:HG22	0.64	1.70	23	14
1:A:8:GLU:OE1	2:B:9:VAL:HG21	0.64	1.92	26	1
1:A:5:LEU:HD23	1:A:8:GLU:OE1	0.64	1.91	9	1
1:A:12:LEU:O	1:A:16:ASN:N	0.63	2.31	18	23
1:A:12:LEU:HD22	2:B:13:LYS:HB2	0.63	1.71	6	2
1:A:8:GLU:HG2	2:B:9:VAL:HG21	0.63	1.69	8	3
1:A:27:GLU:HB3	2:B:26:LEU:HD22	0.62	1.70	26	6
1:A:22:GLU:OE1	1:A:26:LEU:HD11	0.62	1.94	8	1
1:A:13:GLU:HG3	2:B:12:LEU:HD13	0.62	1.71	18	2
2:B:5:LEU:HD23	2:B:8:ARG:CD	0.62	2.24	7	2
1:A:23:VAL:HG22	2:B:23:VAL:HG22	0.62	1.69	16	6
2:B:19:LEU:N	2:B:19:LEU:HD23	0.61	2.09	9	9
1:A:22:GLU:CD	1:A:26:LEU:HD11	0.61	2.16	8	1
1:A:5:LEU:HD22	2:B:6:LYS:HD3	0.61	1.70	11	3
1:A:26:LEU:HD13	2:B:26:LEU:HB2	0.61	1.73	15	1
1:A:5:LEU:HD13	2:B:6:LYS:HB2	0.60	1.72	26	13
1:A:5:LEU:HD12	2:B:5:LEU:HB2	0.60	1.72	1	1
1:A:9:VAL:HG13	2:B:12:LEU:HD11	0.60	1.72	7	12
2:B:15:ARG:HD2	2:B:19:LEU:HD21	0.59	1.72	15	1
1:A:5:LEU:CD1	2:B:6:LYS:N	0.59	2.65	1	1
1:A:5:LEU:HD21	2:B:6:LYS:HB2	0.58	1.75	24	2
2:B:15:ARG:HD2	2:B:19:LEU:HD11	0.58	1.75	15	1
1:A:9:VAL:HG11	2:B:8:ARG:NH2	0.58	2.13	22	1
2:B:22:LYS:HD3	2:B:26:LEU:HD11	0.57	1.76	5	9
1:A:26:LEU:HD22	2:B:27:ARG:HA	0.57	1.77	7	2
1:A:27:GLU:HG2	2:B:26:LEU:HD13	0.57	1.76	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:10:GLN:O	2:B:14:ALA:CB	0.57	2.52	6	14
1:A:12:LEU:HD13	2:B:13:LYS:HB2	0.57	1.76	6	2
2:B:19:LEU:HA	2:B:22:LYS:HG2	0.57	1.75	24	3
1:A:6:GLU:HA	2:B:5:LEU:HD13	0.56	1.76	21	1
1:A:16:ASN:OD1	2:B:16:ASN:CB	0.56	2.53	24	1
1:A:8:GLU:HG2	2:B:9:VAL:HG11	0.56	1.78	7	17
1:A:5:LEU:HD22	2:B:6:LYS:HA	0.56	1.77	22	3
1:A:14:ALA:HB3	1:A:15:GLU:OE1	0.56	2.01	6	1
2:B:13:LYS:HA	2:B:16:ASN:HB3	0.56	1.76	6	2
1:A:23:VAL:HG13	2:B:26:LEU:HD12	0.55	1.77	4	8
1:A:27:GLU:CG	2:B:26:LEU:HD13	0.55	2.31	15	1
2:B:10:GLN:O	2:B:14:ALA:HB3	0.54	2.02	24	2
2:B:5:LEU:HA	2:B:8:ARG:HG2	0.53	1.79	17	9
1:A:9:VAL:HG12	1:A:13:GLU:OE1	0.53	2.04	7	3
1:A:26:LEU:HD13	2:B:26:LEU:CB	0.53	2.33	15	1
1:A:23:VAL:HG13	2:B:26:LEU:HD11	0.53	1.81	15	5
1:A:9:VAL:HG21	2:B:5:LEU:HD22	0.53	1.81	7	4
2:B:19:LEU:HA	2:B:22:LYS:CG	0.53	2.34	9	1
1:A:9:VAL:HG12	1:A:13:GLU:OE2	0.52	2.04	9	1
1:A:16:ASN:ND2	2:B:12:LEU:O	0.52	2.43	24	2
1:A:9:VAL:HG21	2:B:8:ARG:HE	0.52	1.62	19	1
1:A:23:VAL:HG12	1:A:27:GLU:CD	0.52	2.25	9	1
1:A:5:LEU:HD11	2:B:6:LYS:HB2	0.51	1.80	1	1
1:A:5:LEU:HD22	2:B:6:LYS:CG	0.51	2.34	2	1
1:A:23:VAL:CG2	2:B:23:VAL:HG22	0.51	2.36	3	3
1:A:8:GLU:O	1:A:12:LEU:HG	0.51	2.06	6	1
1:A:27:GLU:HB3	2:B:26:LEU:HD13	0.51	1.83	14	4
1:A:9:VAL:HG23	2:B:9:VAL:HG22	0.50	1.82	9	5
2:B:3:GLN:O	2:B:7:LYS:CG	0.50	2.59	5	1
1:A:12:LEU:HD13	2:B:9:VAL:O	0.50	2.06	6	1
1:A:6:GLU:OE1	2:B:5:LEU:HD11	0.49	2.07	21	1
2:B:5:LEU:HD23	2:B:8:ARG:HG2	0.49	1.84	20	5
1:A:12:LEU:CD2	2:B:13:LYS:HD3	0.49	2.36	6	2
1:A:19:LEU:HD11	2:B:20:LYS:CD	0.49	2.38	15	3
1:A:12:LEU:HD22	2:B:13:LYS:CB	0.49	2.38	18	2
1:A:8:GLU:CG	2:B:9:VAL:HG11	0.48	2.38	4	4
1:A:26:LEU:HD22	2:B:27:ARG:HB3	0.48	1.84	12	6
2:B:10:GLN:O	2:B:14:ALA:N	0.48	2.46	6	1
2:B:13:LYS:HD2	2:B:16:ASN:ND2	0.48	2.24	18	1
1:A:12:LEU:CB	2:B:12:LEU:HB2	0.47	2.39	18	1
1:A:9:VAL:HG11	2:B:8:ARG:HH21	0.47	1.69	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:19:LEU:O	2:B:23:VAL:N	0.47	2.42	12	8
1:A:12:LEU:HD22	2:B:13:LYS:CG	0.47	2.40	6	2
1:A:6:GLU:OE2	2:B:5:LEU:HD11	0.47	2.10	9	1
1:A:5:LEU:CD2	2:B:6:LYS:HB2	0.47	2.40	24	2
1:A:19:LEU:HD22	2:B:23:VAL:HG11	0.46	1.87	9	1
1:A:19:LEU:HD11	2:B:20:LYS:HG3	0.46	1.87	19	3
1:A:5:LEU:O	1:A:8:GLU:N	0.46	2.48	24	1
1:A:5:LEU:HD22	2:B:6:LYS:HD2	0.46	1.86	5	1
1:A:12:LEU:HD12	2:B:9:VAL:HG13	0.46	1.87	16	4
1:A:19:LEU:C	1:A:23:VAL:HG23	0.46	2.31	8	1
2:B:3:GLN:HA	2:B:6:LYS:HB3	0.45	1.87	19	2
1:A:19:LEU:O	1:A:23:VAL:CG2	0.45	2.61	24	1
1:A:12:LEU:O	1:A:15:GLU:N	0.45	2.49	24	1
1:A:9:VAL:HG12	1:A:10:ALA:N	0.45	2.25	6	1
2:B:19:LEU:O	2:B:22:LYS:HG3	0.45	2.11	9	1
2:B:22:LYS:CD	2:B:26:LEU:HD11	0.45	2.42	4	2
2:B:12:LEU:O	2:B:16:ASN:CB	0.45	2.65	8	1
1:A:12:LEU:HD13	2:B:13:LYS:H	0.45	1.72	18	2
2:B:8:ARG:O	2:B:11:ALA:HB3	0.45	2.12	24	1
2:B:24:GLN:HA	2:B:27:ARG:HD3	0.44	1.89	13	2
2:B:19:LEU:O	2:B:23:VAL:CG2	0.44	2.65	6	7
2:B:15:ARG:O	2:B:19:LEU:HG	0.44	2.13	15	1
1:A:24:ALA:HB3	1:A:25:GLN:OE1	0.44	2.12	25	1
1:A:9:VAL:HG21	2:B:8:ARG:CD	0.44	2.43	18	1
1:A:6:GLU:CG	2:B:5:LEU:HD13	0.44	2.39	17	1
1:A:19:LEU:HD11	2:B:20:LYS:CE	0.44	2.42	6	1
1:A:5:LEU:HD22	2:B:6:LYS:HG3	0.44	1.89	2	1
2:B:19:LEU:HD23	2:B:19:LEU:N	0.43	2.28	12	5
1:A:9:VAL:HG13	2:B:12:LEU:CD1	0.43	2.43	18	2
1:A:19:LEU:HD22	2:B:23:VAL:HG22	0.43	1.89	24	1
2:B:24:GLN:HA	2:B:27:ARG:CD	0.43	2.43	13	1
1:A:27:GLU:CD	2:B:26:LEU:HD22	0.43	2.34	15	1
2:B:5:LEU:HD23	2:B:8:ARG:NE	0.43	2.28	1	3
1:A:19:LEU:HD22	2:B:23:VAL:HG21	0.43	1.90	12	5
1:A:16:ASN:ND2	2:B:12:LEU:CA	0.43	2.82	24	1
1:A:12:LEU:HD23	1:A:12:LEU:N	0.43	2.29	18	1
2:B:15:ARG:HD3	2:B:19:LEU:HD21	0.42	1.91	18	1
1:A:5:LEU:HD12	2:B:5:LEU:CB	0.42	2.41	1	1
1:A:12:LEU:CD1	2:B:9:VAL:HA	0.42	2.44	18	1
2:B:15:ARG:HD3	2:B:19:LEU:CD1	0.42	2.45	10	1
2:B:15:ARG:HG3	2:B:19:LEU:HD21	0.42	1.90	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:O	1:A:14:ALA:N	0.42	2.53	24	1
2:B:19:LEU:N	2:B:19:LEU:CD2	0.41	2.79	9	1
1:A:7:LYS:CD	1:A:7:LYS:N	0.41	2.84	24	1
1:A:5:LEU:HD22	2:B:6:LYS:CB	0.41	2.46	25	1
1:A:12:LEU:CD1	2:B:9:VAL:O	0.41	2.68	6	1
2:B:22:LYS:NZ	2:B:26:LEU:CD1	0.41	2.83	9	1
1:A:9:VAL:HG21	2:B:5:LEU:CD2	0.41	2.46	15	1
1:A:23:VAL:HG12	1:A:27:GLU:HG2	0.41	1.92	4	2
1:A:12:LEU:HD13	2:B:13:LYS:N	0.41	2.31	8	1
1:A:12:LEU:O	1:A:13:GLU:C	0.41	2.58	24	1
2:B:22:LYS:O	2:B:23:VAL:C	0.40	2.59	16	1
2:B:24:GLN:O	2:B:27:ARG:NE	0.40	2.54	13	1
2:B:19:LEU:O	2:B:22:LYS:N	0.40	2.53	16	1
1:A:16:ASN:ND2	2:B:12:LEU:HA	0.40	2.32	24	1
2:B:22:LYS:O	2:B:25:ALA:N	0.40	2.54	16	1
1:A:17:TYR:CE1	1:A:21:GLN:OE1	0.40	2.74	23	1
1:A:19:LEU:HA	1:A:22:GLU:HG2	0.40	1.91	8	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	23/32 (72%)	21±1 (93±6%)	2±1 (7±6%)	0±0 (0±1%)	50	82
2	B	25/32 (78%)	22±1 (87±5%)	3±1 (12±5%)	0±0 (1±2%)	21	69
All	All	1296/1728 (75%)	1167 (90%)	122 (9%)	7 (1%)	32	76

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)
2	B	3	GLN	3
2	B	23	VAL	3
1	A	13	GLU	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	20/25 (80%)	16±2 (82±9%)	4±2 (18±9%)	4 38
2	B	20/24 (83%)	12±1 (58±7%)	8±1 (42±7%)	0 4
All	All	1080/1323 (82%)	759 (70%)	321 (30%)	1 17

All 27 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)
2	B	8	ARG	27
2	B	13	LYS	25
2	B	12	LEU	24
2	B	22	LYS	24
2	B	19	LEU	23
2	B	27	ARG	23
1	A	21	GLN	19
1	A	27	GLU	16
2	B	7	LYS	15
2	B	20	LYS	13
1	A	7	LYS	12
2	B	15	ARG	12
2	B	6	LYS	11
1	A	18	GLN	10
2	B	10	GLN	9
2	B	3	GLN	8
1	A	11	GLN	8
1	A	15	GLU	8
2	B	21	GLN	8
1	A	22	GLU	8
1	A	20	GLU	6
2	B	24	GLN	3
1	A	25	GLN	3
1	A	12	LEU	2
1	A	6	GLU	2
1	A	8	GLU	1
1	A	16	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