Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 04:26 PM EDT

PDB ID	:	2L42
Title	:	The solution structure of Rap1 BRCT domain from Saccharomyces cerevisiae
Authors	:	Zhang, W.; Zhang, J.; Tu, X.
Deposited on	:	2010-09-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

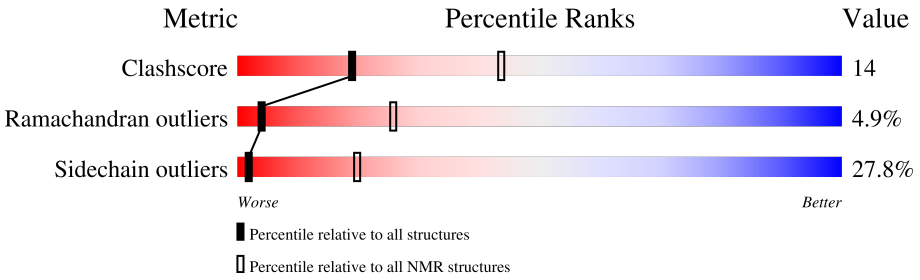
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	106	40% 33% • 17% 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:11-A:20, A:26-A:94 (79)	0.98	15

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1519 atoms, of which 750 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein RAP1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	97	1519	478	750	133	154	4	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P11938
A	98	LEU	-	expression tag	UNP P11938
A	99	GLU	-	expression tag	UNP P11938
A	100	HIS	-	expression tag	UNP P11938
A	101	HIS	-	expression tag	UNP P11938
A	102	HIS	-	expression tag	UNP P11938
A	103	HIS	-	expression tag	UNP P11938
A	104	HIS	-	expression tag	UNP P11938
A	105	HIS	-	expression tag	UNP P11938

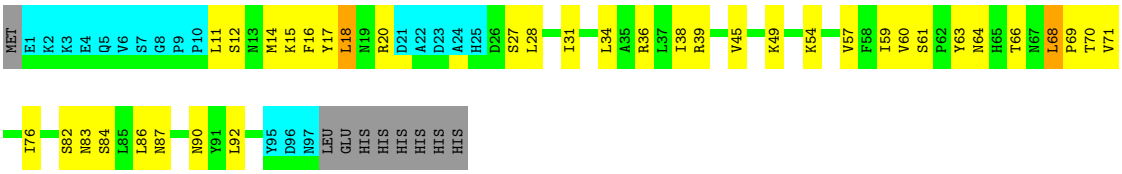
4 Residue-property plots (i)

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: DNA-binding protein RAP1

Chain A: 40% 33% • 17% 8%



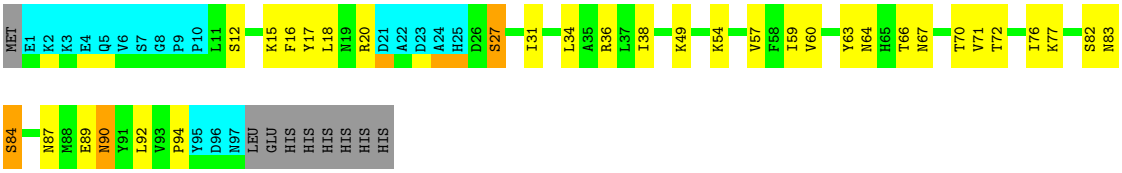
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DNA-binding protein RAP1

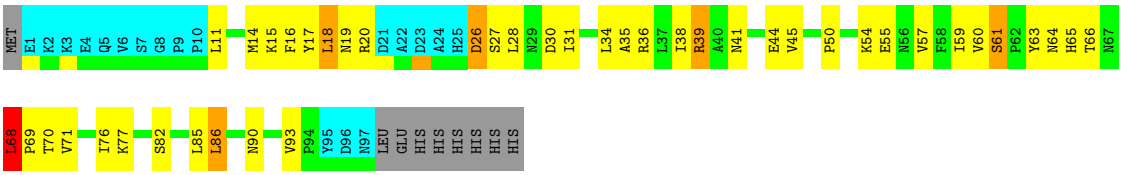
Chain A: 43% 28% • 17% 8%



4.2.2 Score per residue for model 2

• Molecule 1: DNA-binding protein RAP1

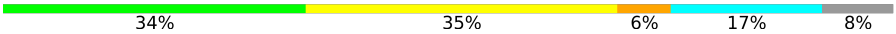
Chain A: 34% 35% 5% • 17% 8%

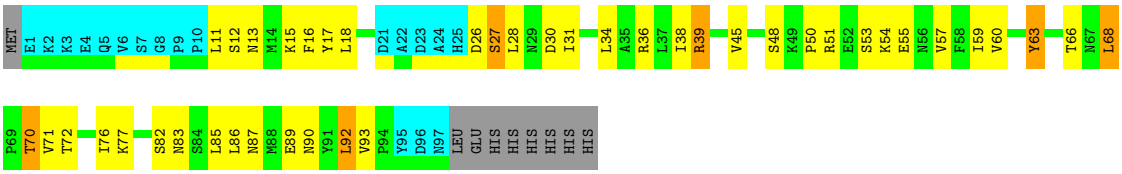


4.2.3 Score per residue for model 3

- Molecule 1: DNA-binding protein RAP1

Chain A:

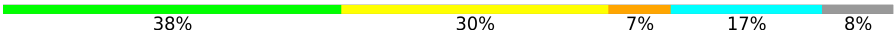


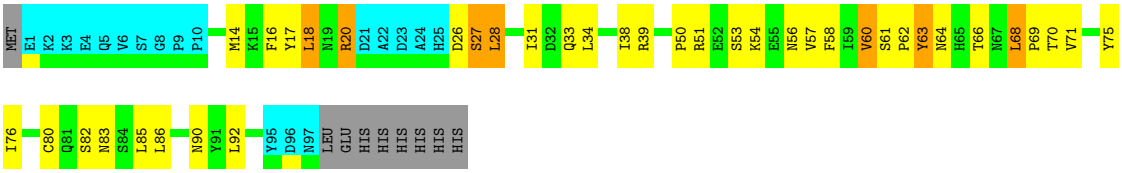


4.2.4 Score per residue for model 4

- Molecule 1: DNA-binding protein RAP1

Chain A:

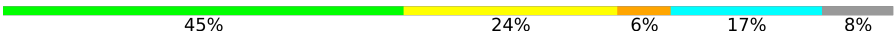


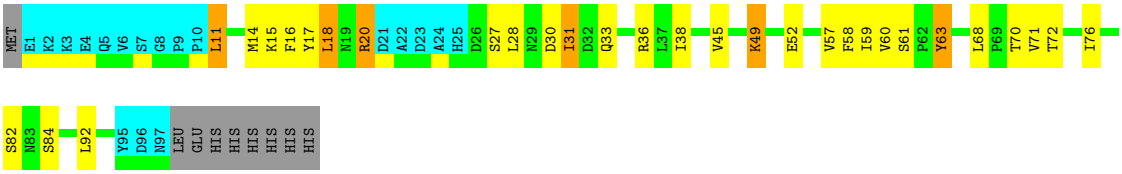


4.2.5 Score per residue for model 5

- Molecule 1: DNA-binding protein RAP1

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: DNA-binding protein RAP1

Chain A: 35% 32% 8% 17% 8%

MET E1 K2 K3 E4 Q5 V6 S7 G8 P9 P10 L11 S12 N13 M14 K15 F16 Y17 L18 D21 A22 D23 A24 H25 D26 S27 D30 I31 L34 I38 R39 A40 N41 V45 S48 K49 K54 E55 N56 V57 F58 I59 V60 S61 P62 Y63 T66 N67 L68 P69 T70 V71

T74 Y75 I76 K77 A78 Q81 S82 N83 S84 L85 L86 N87 M88 E89 L92 Y95 D96 N97 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.7 Score per residue for model 7

- Molecule 1: DNA-binding protein RAP1

Chain A: 37% 28% 9% 17% 8%

MET E1 K2 K3 E4 Q5 V6 S7 G8 P9 P10 L11 S12 N13 M14 K15 F16 Y17 L18 N19 R20 D21 A22 D23 A24 H25 D26 S27 L28 N29 D30 I31 L34 I38 N41 G42 G43 E44 V45 K49 P50 R51 E55 N56 V57 F58 I59 V60 S61 P62 Y63 L68 V71

T72 P73 T74 Y75 I76 K77 S82 N83 S84 N87 M88 L92 Y95 D96 N97 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.8 Score per residue for model 8

- Molecule 1: DNA-binding protein RAP1

Chain A: 34% 35% 6% 17% 8%

MET E1 K2 K3 E4 Q5 V6 S7 G8 P9 P10 L11 S12 N13 M14 K15 F16 Y17 L18 D21 A22 D23 A24 H25 D26 S27 I31 L34 A35 R36 L37 I38 R39 V45 L46 D47 S48 K49 P50 R51 E52 S53 K54 E55 N56 V57 F58 I59 V60 S61 P62 Y63 N64 H65 L68

P69 T70 V71 Y75 I76 K77 A78 C79 C80 N83 S84 L85 L86 N87 M88 E89 N90 Y91 L92 Y95 D96 N97 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.9 Score per residue for model 9

- Molecule 1: DNA-binding protein RAP1

Chain A: 35% 37% • 17% 8%

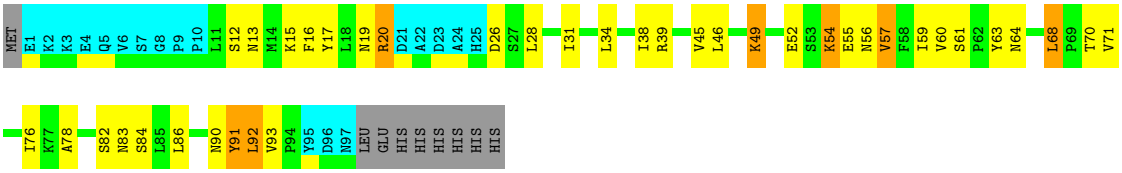
MET E1 K2 K3 E4 Q5 V6 S7 G8 P9 P10 L11 S12 N13 F16 Y17 L18 N19 R20 D21 A22 D23 A24 H25 D26 S27 L28 N29 D30 I31 L34 A35 R36 R39 V45 S48 K49 P50 K54 E55 N56 V57 F58 I59 V60 S61 P62 Y63 T66 N67 L68 P69 T70

V71 T72 P73 T74 Y75 I76 K77 S82 N83 S84 L85 L86 N87 M88 E89 N90 Y95 D96 N97 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.10 Score per residue for model 10

- Molecule 1: DNA-binding protein RAP1

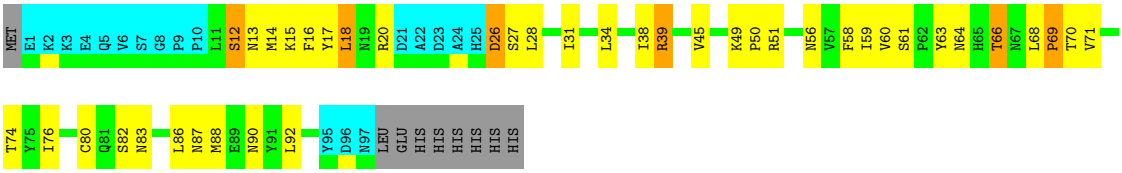
Chain A: 38% 30% 7% 17% 8%



4.2.11 Score per residue for model 11

- Molecule 1: DNA-binding protein RAP1

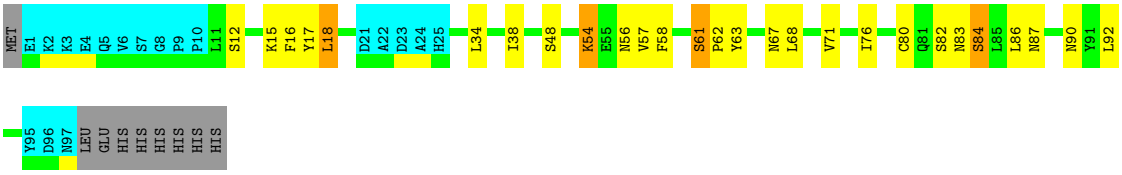
Chain A: 36% 33% 6% 17% 8%



4.2.12 Score per residue for model 12

- Molecule 1: DNA-binding protein RAP1

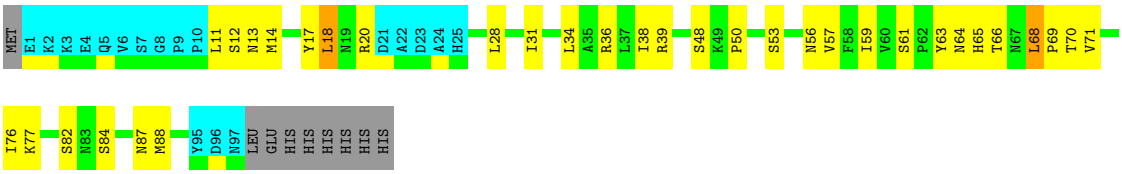
Chain A: 49% 22% • 17% 8%



4.2.13 Score per residue for model 13

- Molecule 1: DNA-binding protein RAP1

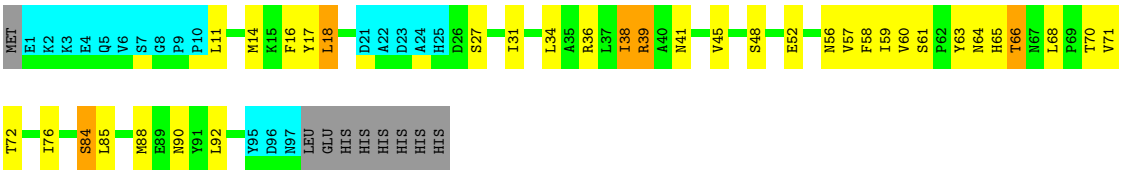
Chain A: 42% 30% • 17% 8%



4.2.14 Score per residue for model 14

- Molecule 1: DNA-binding protein RAP1

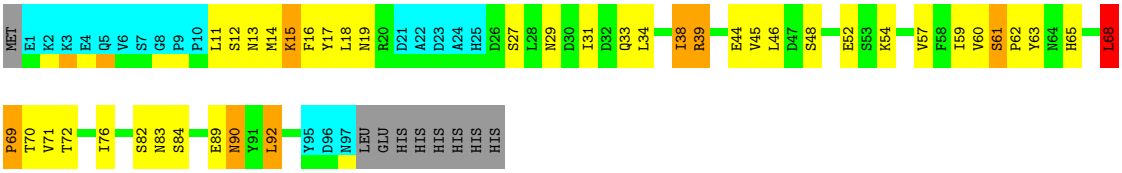
Chain A: 42% 28% 5% 17% 8%



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: DNA-binding protein RAP1

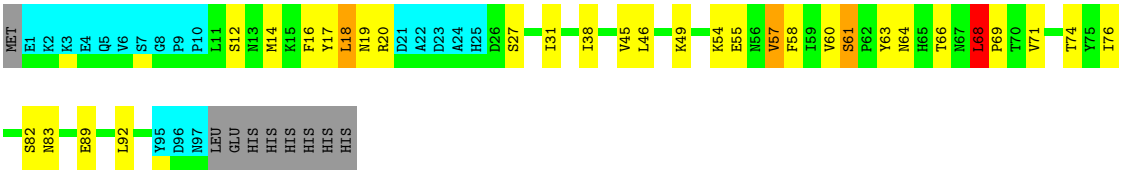
Chain A: 36% 31% 7% • 17% 8%



4.2.16 Score per residue for model 16

- Molecule 1: DNA-binding protein RAP1

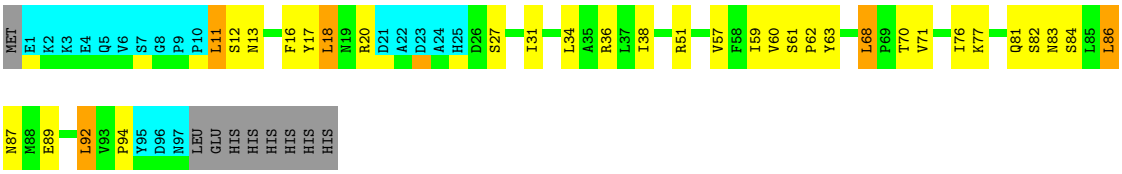
Chain A: 45% 25% • • 17% 8%



4.2.17 Score per residue for model 17

- Molecule 1: DNA-binding protein RAP1

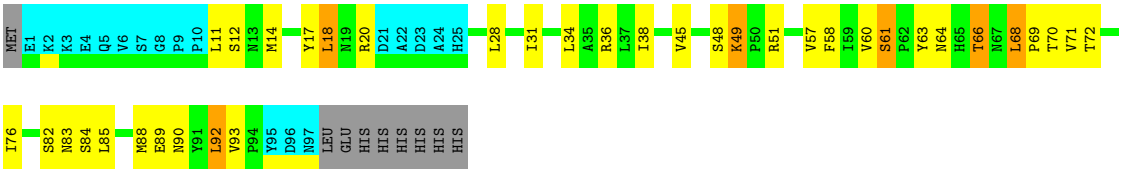
Chain A: 43% 26% 5% 17% 8%



4.2.18 Score per residue for model 18

- Molecule 1: DNA-binding protein RAP1

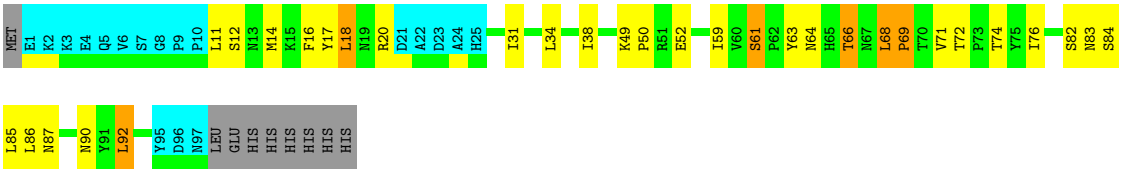
Chain A: 40% 29% 6% 17% 8%



4.2.19 Score per residue for model 19

- Molecule 1: DNA-binding protein RAP1

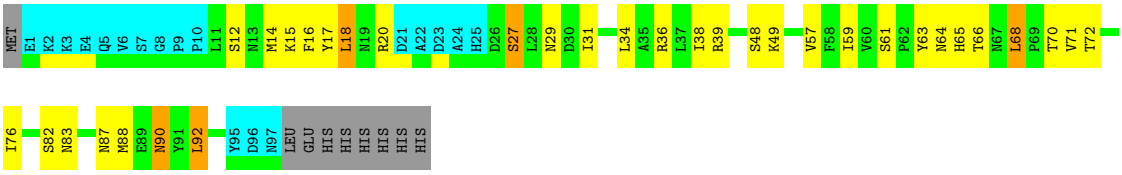
Chain A: 44% 25% 6% 17% 8%



4.2.20 Score per residue for model 20

- Molecule 1: DNA-binding protein RAP1

Chain A: 42% 27% 5% 17% 8%



5 Refinement protocol and experimental data overview (i)

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

Of the 150 calculated structures, 20 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
CNS	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	629	628	627	18±4
All	All	12580	12560	12540	358

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 14.

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:LEU:HD23	1:A:57:VAL:HG12	1.01	1.29	17	7
1:A:38:ILE:HD12	1:A:76:ILE:HD12	0.81	1.51	1	1
1:A:38:ILE:HG13	1:A:76:ILE:HD12	0.80	1.52	8	2
1:A:34:LEU:HD12	1:A:76:ILE:HD12	0.78	1.55	3	1
1:A:39:ARG:HB3	1:A:45:VAL:HG12	0.77	1.55	2	2
1:A:18:LEU:CD2	1:A:57:VAL:HG12	0.75	2.11	12	8
1:A:71:VAL:HG12	1:A:92:LEU:HB3	0.74	1.58	8	7
1:A:16:PHE:CE1	1:A:18:LEU:HD13	0.73	2.19	4	5
1:A:61:SER:HB3	1:A:71:VAL:HG21	0.72	1.61	9	5
1:A:61:SER:HB3	1:A:71:VAL:HG11	0.71	1.60	16	1
1:A:61:SER:HB2	1:A:71:VAL:HG11	0.71	1.63	12	3
1:A:28:LEU:HD12	1:A:49:LYS:HB3	0.70	1.60	10	1
1:A:61:SER:HB2	1:A:71:VAL:HG21	0.70	1.63	19	3
1:A:27:SER:HB3	1:A:31:ILE:HG23	0.68	1.64	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ALA:HB1	1:A:86:LEU:HB2	0.68	1.63	10	2
1:A:38:ILE:HD13	1:A:76:ILE:HD12	0.68	1.66	4	2
1:A:34:LEU:CD1	1:A:76:ILE:HD12	0.66	2.20	3	5
1:A:27:SER:CB	1:A:31:ILE:HG23	0.66	2.20	7	3
1:A:34:LEU:HD13	1:A:76:ILE:HB	0.63	1.70	12	6
1:A:38:ILE:CD1	1:A:76:ILE:HG23	0.63	2.23	10	11
1:A:11:LEU:HD21	1:A:41:ASN:ND2	0.63	2.09	6	1
1:A:28:LEU:HD22	1:A:49:LYS:HG3	0.63	1.69	7	1
1:A:28:LEU:HD22	1:A:31:ILE:HD11	0.62	1.68	4	1
1:A:18:LEU:HD23	1:A:57:VAL:CG1	0.61	2.26	18	5
1:A:38:ILE:HD12	1:A:76:ILE:CD1	0.61	2.23	1	1
1:A:90:ASN:HB3	1:A:92:LEU:HD23	0.60	1.73	15	5
1:A:61:SER:CB	1:A:71:VAL:HG21	0.60	2.26	6	7
1:A:17:TYR:CE2	1:A:31:ILE:HD12	0.60	2.32	4	2
1:A:18:LEU:HD23	1:A:57:VAL:HA	0.60	1.74	15	4
1:A:70:THR:HB	1:A:93:VAL:HG23	0.59	1.72	18	2
1:A:18:LEU:HD22	1:A:57:VAL:HG12	0.59	1.74	5	1
1:A:17:TYR:HD2	1:A:31:ILE:HD12	0.59	1.56	9	9
1:A:70:THR:N	1:A:93:VAL:HG12	0.59	2.11	10	2
1:A:92:LEU:O	1:A:92:LEU:HD12	0.59	1.98	17	2
1:A:18:LEU:HD12	1:A:48:SER:HB3	0.59	1.73	15	1
1:A:34:LEU:HD11	1:A:76:ILE:HD12	0.58	1.74	2	2
1:A:78:ALA:HB1	1:A:86:LEU:CB	0.58	2.28	10	1
1:A:38:ILE:HG13	1:A:76:ILE:HD13	0.58	1.75	17	3
1:A:35:ALA:HB1	1:A:45:VAL:HG11	0.58	1.74	2	1
1:A:38:ILE:HD13	1:A:76:ILE:HG23	0.57	1.75	15	2
1:A:61:SER:CB	1:A:71:VAL:HG11	0.56	2.30	16	3
1:A:39:ARG:HB2	1:A:45:VAL:HG12	0.56	1.77	6	4
1:A:38:ILE:HD11	1:A:76:ILE:HG23	0.56	1.75	10	5
1:A:31:ILE:HG22	1:A:34:LEU:HD21	0.56	1.77	3	6
1:A:60:VAL:HG11	1:A:67:ASN:OD1	0.56	2.01	1	1
1:A:92:LEU:HD12	1:A:92:LEU:O	0.56	2.00	4	2
1:A:28:LEU:HD22	1:A:50:PRO:HD3	0.56	1.78	2	1
1:A:66:THR:HG22	1:A:68:LEU:HD13	0.55	1.78	19	1
1:A:38:ILE:HG12	1:A:76:ILE:HD12	0.55	1.77	7	1
1:A:34:LEU:CD1	1:A:76:ILE:HG21	0.55	2.31	18	6
1:A:68:LEU:N	1:A:69:PRO:CD	0.54	2.70	18	1
1:A:17:TYR:CD2	1:A:31:ILE:HD12	0.54	2.37	16	13
1:A:34:LEU:HD12	1:A:76:ILE:HG21	0.54	1.80	14	5
1:A:61:SER:OG	1:A:71:VAL:HG21	0.54	2.03	14	2
1:A:78:ALA:HB1	1:A:86:LEU:CD2	0.54	2.32	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:TYR:O	1:A:18:LEU:HD12	0.54	2.03	4	8
1:A:15:LYS:NZ	1:A:76:ILE:HD11	0.54	2.17	5	1
1:A:28:LEU:HD23	1:A:50:PRO:HD2	0.54	1.78	3	1
1:A:28:LEU:O	1:A:28:LEU:HD13	0.53	2.03	4	1
1:A:16:PHE:CZ	1:A:18:LEU:HB2	0.52	2.39	9	1
1:A:18:LEU:O	1:A:57:VAL:HB	0.52	2.03	15	2
1:A:16:PHE:CZ	1:A:18:LEU:HD22	0.52	2.39	15	5
1:A:59:ILE:H	1:A:70:THR:HG23	0.52	1.65	1	11
1:A:17:TYR:CE1	1:A:59:ILE:HD11	0.52	2.40	7	3
1:A:28:LEU:HD13	1:A:50:PRO:HD2	0.51	1.82	13	2
1:A:38:ILE:HD13	1:A:76:ILE:CG2	0.51	2.35	11	3
1:A:38:ILE:HG12	1:A:76:ILE:HG23	0.51	1.81	19	2
1:A:16:PHE:CZ	1:A:18:LEU:HD13	0.51	2.41	19	3
1:A:68:LEU:CB	1:A:69:PRO:HD3	0.50	2.36	13	3
1:A:38:ILE:HD12	1:A:38:ILE:N	0.50	2.22	6	5
1:A:70:THR:H	1:A:93:VAL:HG12	0.50	1.67	10	2
1:A:70:THR:HB	1:A:93:VAL:CG2	0.50	2.37	18	1
1:A:16:PHE:HZ	1:A:18:LEU:HD22	0.49	1.67	8	7
1:A:20:ARG:HA	1:A:57:VAL:HG23	0.49	1.84	18	5
1:A:17:TYR:CD1	1:A:45:VAL:CG2	0.49	2.96	7	6
1:A:68:LEU:CB	1:A:69:PRO:CD	0.49	2.91	15	5
1:A:85:LEU:HB3	1:A:86:LEU:HD12	0.49	1.83	3	1
1:A:34:LEU:HD13	1:A:76:ILE:HG21	0.48	1.85	9	2
1:A:59:ILE:HG23	1:A:71:VAL:O	0.48	2.09	14	5
1:A:70:THR:O	1:A:92:LEU:HA	0.48	2.08	17	3
1:A:16:PHE:HB3	1:A:60:VAL:HG22	0.48	1.84	5	3
1:A:11:LEU:HD23	1:A:41:ASN:ND2	0.48	2.23	14	1
1:A:61:SER:OG	1:A:71:VAL:HG11	0.47	2.09	13	3
1:A:17:TYR:CZ	1:A:59:ILE:HD11	0.47	2.44	17	6
1:A:16:PHE:CB	1:A:60:VAL:HG22	0.47	2.38	5	1
1:A:20:ARG:HG2	1:A:57:VAL:HG23	0.47	1.86	7	2
1:A:34:LEU:C	1:A:34:LEU:HD12	0.47	2.30	12	5
1:A:28:LEU:HD22	1:A:49:LYS:CB	0.47	2.40	5	1
1:A:54:LYS:HE3	1:A:57:VAL:HG13	0.47	1.87	10	1
1:A:59:ILE:O	1:A:71:VAL:HG22	0.46	2.11	8	2
1:A:28:LEU:HD13	1:A:49:LYS:HG2	0.46	1.87	18	1
1:A:66:THR:HG22	1:A:69:PRO:HD3	0.46	1.86	11	1
1:A:27:SER:O	1:A:31:ILE:HG23	0.45	2.11	4	1
1:A:18:LEU:HD12	1:A:57:VAL:HG12	0.45	1.88	6	1
1:A:38:ILE:O	1:A:41:ASN:ND2	0.45	2.50	7	1
1:A:16:PHE:N	1:A:60:VAL:HG22	0.45	2.26	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:PHE:O	1:A:59:ILE:HA	0.45	2.11	9	1
1:A:62:PRO:O	1:A:63:TYR:CB	0.45	2.64	17	4
1:A:68:LEU:N	1:A:69:PRO:HD2	0.44	2.27	18	1
1:A:85:LEU:C	1:A:86:LEU:HD23	0.44	2.33	2	1
1:A:11:LEU:CD1	1:A:38:ILE:HG23	0.44	2.42	6	2
1:A:15:LYS:HE3	1:A:38:ILE:HG21	0.44	1.88	5	1
1:A:68:LEU:HB3	1:A:69:PRO:HD3	0.44	1.88	2	1
1:A:28:LEU:HD13	1:A:50:PRO:CD	0.44	2.43	2	1
1:A:38:ILE:CD1	1:A:76:ILE:HD12	0.43	2.41	4	1
1:A:15:LYS:CE	1:A:38:ILE:HG21	0.43	2.43	2	1
1:A:70:THR:O	1:A:92:LEU:CB	0.43	2.67	10	1
1:A:14:MET:O	1:A:62:PRO:HA	0.43	2.14	4	1
1:A:28:LEU:HA	1:A:31:ILE:HD11	0.42	1.91	2	1
1:A:39:ARG:HG3	1:A:45:VAL:HG12	0.42	1.90	10	1
1:A:27:SER:HB2	1:A:31:ILE:HG23	0.42	1.90	7	1
1:A:54:LYS:HG3	1:A:56:ASN:HB2	0.42	1.90	12	2
1:A:16:PHE:CE1	1:A:18:LEU:HD23	0.42	2.50	6	1
1:A:92:LEU:HD12	1:A:92:LEU:C	0.42	2.34	11	1
1:A:17:TYR:CD1	1:A:45:VAL:HG21	0.42	2.50	3	1
1:A:38:ILE:CG1	1:A:76:ILE:HG23	0.42	2.44	19	1
1:A:78:ALA:HB1	1:A:86:LEU:HD22	0.42	1.90	6	1
1:A:39:ARG:CG	1:A:45:VAL:HG12	0.42	2.44	9	1
1:A:15:LYS:HE2	1:A:38:ILE:CG2	0.41	2.45	1	1
1:A:38:ILE:HD12	1:A:76:ILE:HG23	0.41	1.92	1	1
1:A:27:SER:HB3	1:A:31:ILE:CG2	0.41	2.45	20	1
1:A:15:LYS:CD	1:A:38:ILE:HG21	0.41	2.46	15	1
1:A:38:ILE:HD13	1:A:76:ILE:CD1	0.41	2.40	15	1
1:A:16:PHE:O	1:A:59:ILE:HG13	0.41	2.16	20	2
1:A:59:ILE:HG23	1:A:59:ILE:O	0.41	2.14	3	1
1:A:28:LEU:HD22	1:A:50:PRO:HD2	0.41	1.92	9	1
1:A:17:TYR:O	1:A:18:LEU:HD22	0.41	2.15	6	1
1:A:78:ALA:HB3	1:A:89:GLU:HG3	0.41	1.92	8	1
1:A:90:ASN:ND2	1:A:92:LEU:HD23	0.41	2.30	11	1
1:A:61:SER:O	1:A:64:ASN:HB2	0.41	2.16	2	1
1:A:45:VAL:O	1:A:46:LEU:HD23	0.41	2.16	16	1
1:A:71:VAL:HG22	1:A:92:LEU:CD1	0.40	2.46	7	1
1:A:11:LEU:HD23	1:A:41:ASN:CG	0.40	2.37	14	1
1:A:17:TYR:CD1	1:A:45:VAL:HG23	0.40	2.51	5	1
1:A:16:PHE:CE2	1:A:18:LEU:HB2	0.40	2.52	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	79/106 (75%)	62±2 (79±2%)	13±2 (16±2%)	4±1 (5±2%)	4 26
All	All	1580/2120 (75%)	1244 (79%)	259 (16%)	77 (5%)	4 26

All 17 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	12	SER	16
1	A	68	LEU	13
1	A	66	THR	9
1	A	84	SER	6
1	A	26	ASP	5
1	A	63	TYR	5
1	A	83	ASN	5
1	A	50	PRO	4
1	A	69	PRO	3
1	A	94	PRO	2
1	A	91	TYR	2
1	A	19	ASN	2
1	A	20	ARG	1
1	A	85	LEU	1
1	A	43	GLY	1
1	A	13	ASN	1
1	A	86	LEU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	74/98 (76%)	53±3 (72±4%)	21±3 (28±4%)	2 20
All	All	1480/1960 (76%)	1068 (72%)	412 (28%)	2 20

All 59 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	82	SER	18
1	A	63	TYR	17
1	A	18	LEU	15
1	A	68	LEU	14
1	A	92	LEU	14
1	A	27	SER	12
1	A	49	LYS	12
1	A	14	MET	12
1	A	36	ARG	11
1	A	87	ASN	11
1	A	11	LEU	11
1	A	54	LYS	10
1	A	64	ASN	10
1	A	72	THR	10
1	A	83	ASN	10
1	A	84	SER	10
1	A	90	ASN	10
1	A	20	ARG	9
1	A	39	ARG	9
1	A	61	SER	9
1	A	15	LYS	9
1	A	48	SER	9
1	A	88	MET	9
1	A	89	GLU	8
1	A	55	GLU	8
1	A	58	PHE	8
1	A	77	LYS	7
1	A	86	LEU	7
1	A	13	ASN	7
1	A	51	ARG	7
1	A	60	VAL	7
1	A	66	THR	7
1	A	65	HIS	6
1	A	52	GLU	6
1	A	74	THR	6
1	A	57	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	30	ASP	5
1	A	85	LEU	5
1	A	56	ASN	5
1	A	26	ASP	4
1	A	70	THR	4
1	A	80	CYS	4
1	A	29	ASN	4
1	A	19	ASN	3
1	A	28	LEU	3
1	A	33	GLN	3
1	A	41	ASN	2
1	A	44	GLU	2
1	A	53	SER	2
1	A	75	TYR	2
1	A	12	SER	2
1	A	81	GLN	2
1	A	91	TYR	2
1	A	46	LEU	2
1	A	38	ILE	2
1	A	31	ILE	1
1	A	37	LEU	1
1	A	47	ASP	1
1	A	67	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