Full wwPDB NMR Structure Validation Report (i)

Mar 7, 2022 – 05:59 AM EST

PDB ID	:	2YS4
Title	:	Solution structure of the N-terminal PapD-like domain of HYDIN protein from human
Authors	:	Li, H.; Tomizawa, T.; Koshiba, S.; Watanabe, S.; Harada, T.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-04-03

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:

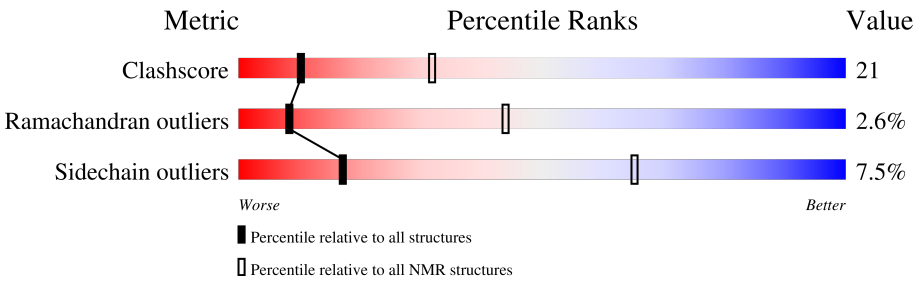
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	122	50% 28% • 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:24-A:120 (97)	0.25	2

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 3 clusters and 7 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1879 atoms, of which 944 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hydrocephalus-inducing protein homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1879	592	944	161	177	5	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q4G0P3
A	2	SER	-	expression tag	UNP Q4G0P3
A	3	SER	-	expression tag	UNP Q4G0P3
A	4	GLY	-	expression tag	UNP Q4G0P3
A	5	SER	-	expression tag	UNP Q4G0P3
A	6	SER	-	expression tag	UNP Q4G0P3
A	7	GLY	-	expression tag	UNP Q4G0P3

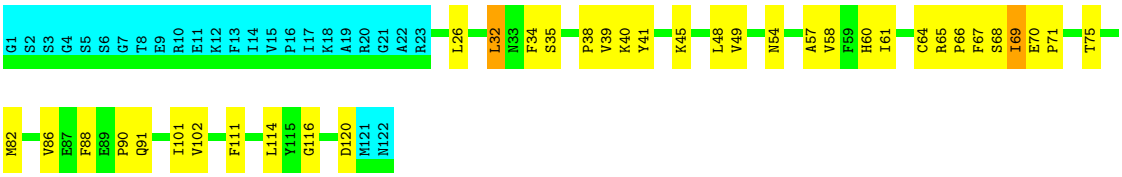
4 Residue-property plots (i)

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: Hydrocephalus-inducing protein homolog

Chain A: 50% 28% • 20%



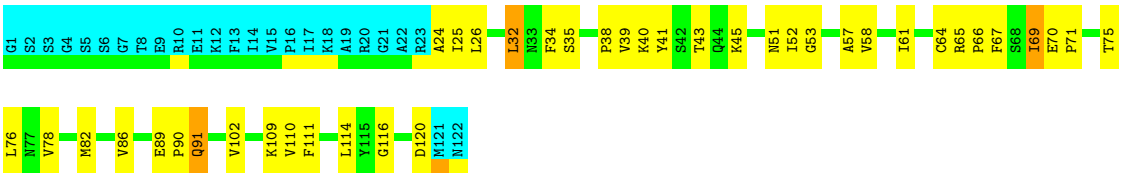
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Hydrocephalus-inducing protein homolog

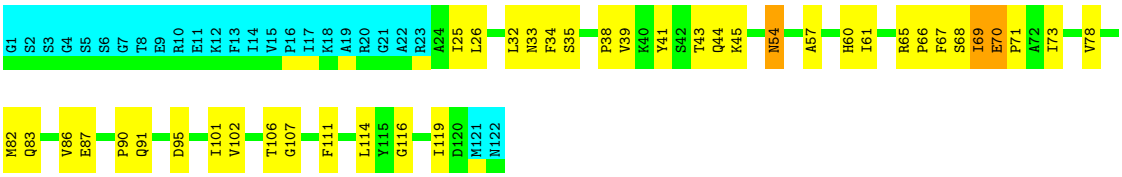
Chain A: 47% 30% • 20%



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Hydrocephalus-inducing protein homolog

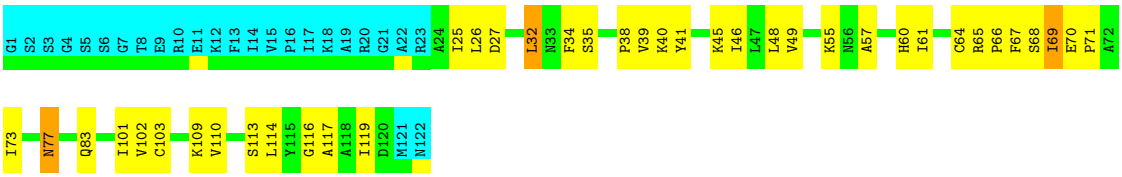
Chain A: 47% 30% • 20%



4.2.3 Score per residue for model 3

- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A:



4.2.4 Score per residue for model 4

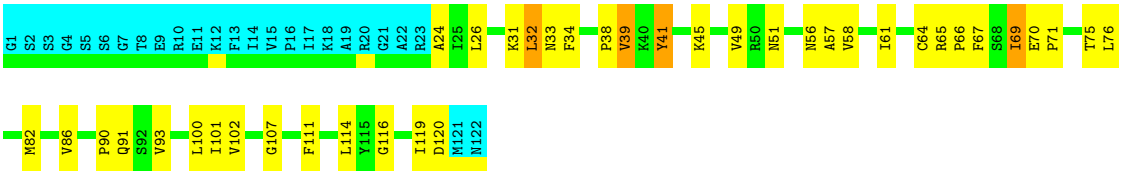
- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A:

4.2.5 Score per residue for model 5

- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A: 48% 27% • 20%

G1 S2 S3 G4 S5 S6 G7 T8 E9 R10 E11 K12 F13 I14 V15 P16 I17 K18 A19 R20 G21 A22 R23 A24 I25 L26 K31 L32 N33 F34 S35 P38 V39 K40 Y41 K45 N51 N54 A57 V58 I61 K62 R65 P66 F67 S68 I69 E70 P71 T75

V78 V86 E87 F88 E89 V102 C103 Y104 D105 T106 G107 V112 S113 L114 Y115 G116 A117 A118 M121 N122

4.2.7 Score per residue for model 7

- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A: 43% 31% 5% 20%

G1 S2 S3 G4 S5 S6 G7 T8 E9 R10 E11 K12 F13 I14 V15 P16 I17 K18 A19 R20 G21 A22 R23 L26 D27 F28 P29 D30 K31 L32 N33 F34 S35 P38 V39 K40 Y41 K45 I46 L47 L48 V49 R50 N51 K55 N56 A57 V58 F59 H60 C64 R65 P66 F67 S68

I69 E70 P71 A72 T73 G74 T75 L76 N77 V78 M82 Q83 L84 E85 V86 E87 F88 E89 P90 Q91 D95 I101 Y104 D105 F111 L114 Y115 G116 A117 A118 M121 N122

4.2.8 Score per residue for model 8

- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A: 48% 27% • 20%

G1 S2 S3 G4 S5 S6 G7 T8 E9 R10 E11 K12 F13 I14 V15 P16 I17 K18 A19 R20 G21 A22 R23 A24 I25 L26 D30 K31 L32 N33 F34 S35 V39 K40 T43 Q44 K45 L48 V49 N54 K55 N56 A57 R65 P66 F67 S68 I69 E70 P71 V78 M82

V86 E87 F88 Q91 I101 V102 T106 K109 V110 F111 G116 D120 M121 N122

4.2.9 Score per residue for model 9

- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A: 52% 26% • 20%

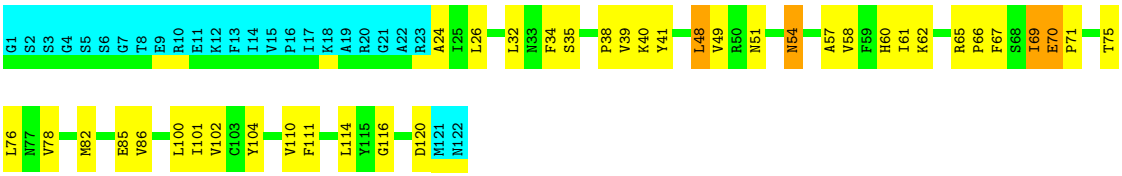
G1 S2 S3 G4 S5 S6 G7 T8 E9 R10 E11 K12 F13 I14 V15 P16 I17 K18 A19 R20 G21 A22 R23 A24 I25 L26 K31 L32 N33 F34 S35 P38 V39 K40 Y41 K45 L48 V49 A57 C64 R65 P66 F67 S68 I69 E70 P71 L76 M82 F88 E89

P90 D95 R99 E108 G116 A117 A118 I119 D120 M121 N122

4.2.10 Score per residue for model 10

- Molecule 1: Hydrocephalus-inducing protein homolog

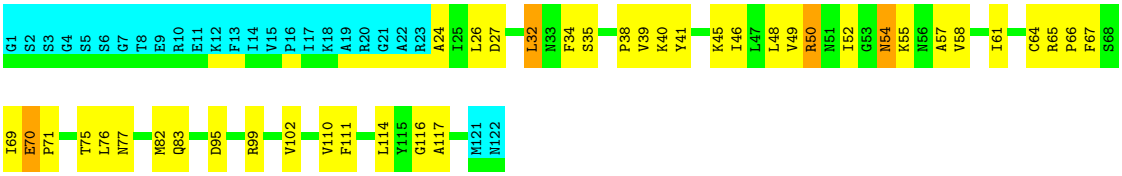
Chain A: 48% 29% • 20%



4.2.11 Score per residue for model 11

- Molecule 1: Hydrocephalus-inducing protein homolog

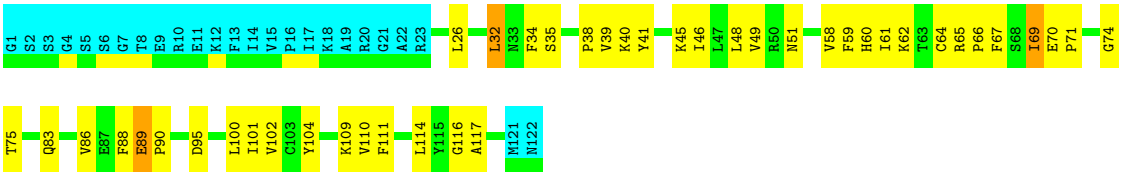
Chain A: 46% 30% • 20%



4.2.12 Score per residue for model 12

- Molecule 1: Hydrocephalus-inducing protein homolog

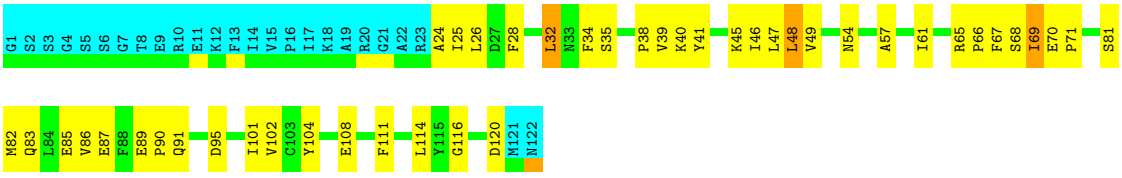
Chain A: 44% 33% • 20%



4.2.13 Score per residue for model 13

- Molecule 1: Hydrocephalus-inducing protein homolog

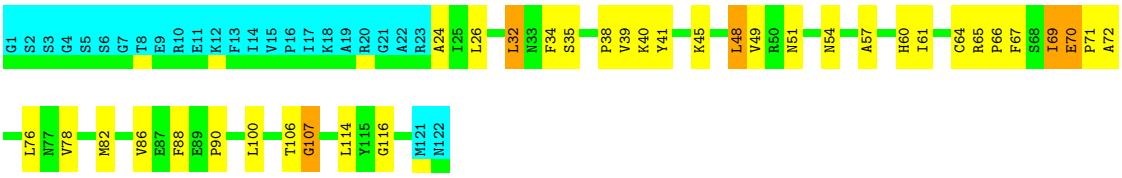
Chain A: 43% 34% • 20%



4.2.14 Score per residue for model 14

• Molecule 1: Hydrocephalus-inducing protein homolog

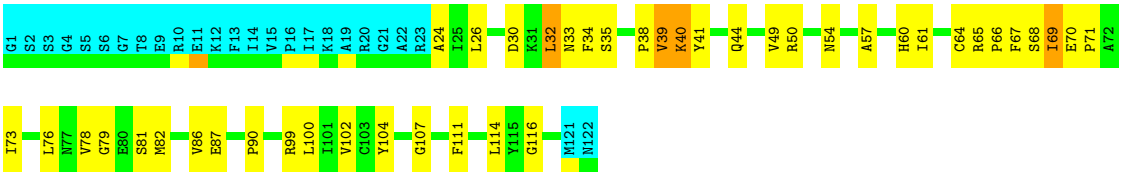
Chain A: 50% 25% • 20%



4.2.15 Score per residue for model 15

• Molecule 1: Hydrocephalus-inducing protein homolog

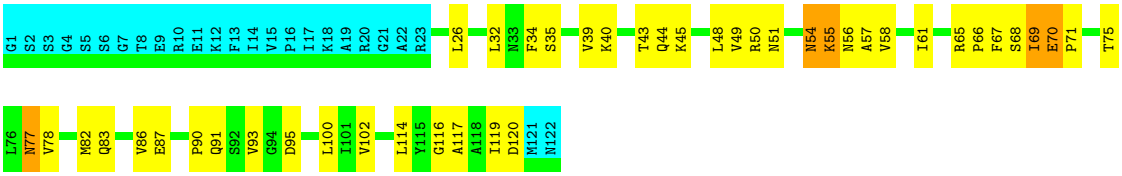
Chain A: 44% 32% • 20%



4.2.16 Score per residue for model 16

• Molecule 1: Hydrocephalus-inducing protein homolog

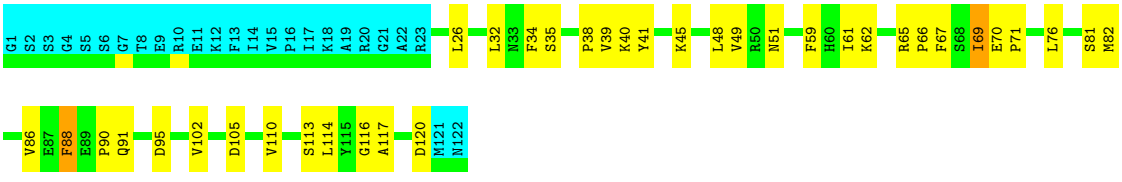
Chain A: 43% 32% • 20%



4.2.17 Score per residue for model 17

• Molecule 1: Hydrocephalus-inducing protein homolog

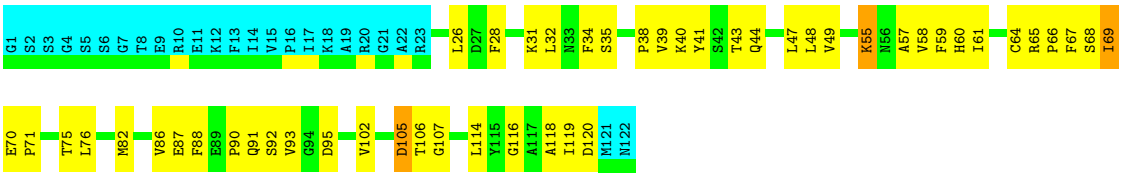
Chain A: 49% 29% • 20%



4.2.18 Score per residue for model 18

- Molecule 1: Hydrocephalus-inducing protein homolog

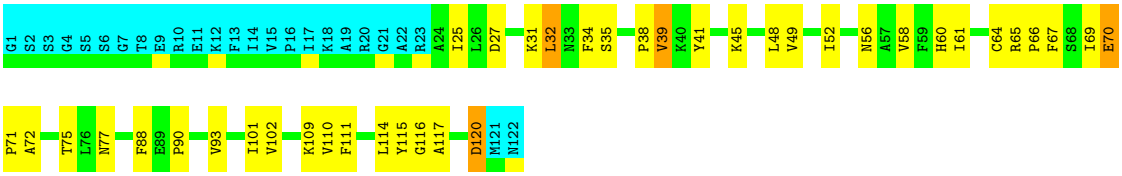
Chain A: 39% 38% • 20%



4.2.19 Score per residue for model 19

- Molecule 1: Hydrocephalus-inducing protein homolog

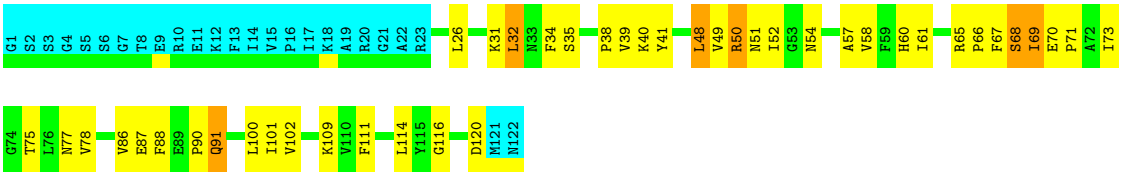
Chain A: 47% 30% • 20%



4.2.20 Score per residue for model 20

- Molecule 1: Hydrocephalus-inducing protein homolog

Chain A: 44% 30% 5% 20%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	752	756	754	32±6
All	All	15040	15120	15080	646

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:PHE:CD1	1:A:114:LEU:HD13	0.90	2.02	17	17
1:A:76:LEU:HD13	1:A:82:MET:SD	0.86	2.11	18	7
1:A:32:LEU:HD12	1:A:34:PHE:CD2	0.84	2.06	12	12
1:A:24:ALA:O	1:A:25:ILE:HD13	0.83	1.73	13	2
1:A:26:LEU:HD21	1:A:57:ALA:CB	0.82	2.05	9	13
1:A:61:ILE:HG12	1:A:102:VAL:HG22	0.77	1.55	16	16
1:A:67:PHE:CZ	1:A:88:PHE:CD1	0.75	2.75	12	1
1:A:26:LEU:HD12	1:A:49:VAL:HG12	0.74	1.57	7	9
1:A:39:VAL:HG11	1:A:93:VAL:HG22	0.74	1.57	19	2
1:A:48:LEU:HD13	1:A:49:VAL:N	0.73	1.98	12	9
1:A:67:PHE:CE2	1:A:88:PHE:CE1	0.73	2.76	12	1
1:A:32:LEU:HD22	1:A:34:PHE:CE1	0.73	2.17	18	3
1:A:26:LEU:HD21	1:A:57:ALA:HB1	0.72	1.61	5	12
1:A:67:PHE:CZ	1:A:88:PHE:CE1	0.72	2.77	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:VAL:HG23	1:A:90:PRO:O	0.72	1.84	20	4
1:A:102:VAL:HB	1:A:110:VAL:HG12	0.71	1.60	10	5
1:A:32:LEU:HD12	1:A:34:PHE:CE1	0.71	2.20	8	3
1:A:67:PHE:CE1	1:A:114:LEU:HD13	0.71	2.20	17	3
1:A:93:VAL:HG21	1:A:120:ASP:HB2	0.71	1.63	5	1
1:A:67:PHE:CE1	1:A:88:PHE:CD1	0.70	2.79	9	6
1:A:32:LEU:HD12	1:A:34:PHE:CD1	0.69	2.22	5	3
1:A:69:ILE:HG22	1:A:86:VAL:HG13	0.68	1.65	15	15
1:A:100:LEU:HD21	1:A:114:LEU:HD11	0.68	1.63	10	1
1:A:32:LEU:HD11	1:A:45:LYS:CE	0.68	2.19	6	3
1:A:58:VAL:HG22	1:A:75:THR:HG22	0.68	1.64	1	9
1:A:39:VAL:HG13	1:A:40:LYS:H	0.68	1.49	20	14
1:A:24:ALA:HB1	1:A:57:ALA:HB2	0.67	1.66	8	5
1:A:100:LEU:CD1	1:A:114:LEU:HD21	0.67	2.20	20	4
1:A:100:LEU:HD11	1:A:114:LEU:HD21	0.66	1.66	16	6
1:A:26:LEU:HD12	1:A:49:VAL:CG1	0.66	2.20	7	7
1:A:34:PHE:CE1	1:A:45:LYS:CD	0.65	2.79	12	1
1:A:32:LEU:HD13	1:A:33:ASN:N	0.65	2.07	6	4
1:A:32:LEU:HD11	1:A:45:LYS:HD2	0.64	1.67	14	1
1:A:58:VAL:HB	1:A:75:THR:HG22	0.64	1.70	7	1
1:A:54:ASN:C	1:A:78:VAL:HG11	0.64	2.13	16	4
1:A:49:VAL:HG21	1:A:84:LEU:CD1	0.63	2.24	7	1
1:A:58:VAL:O	1:A:104:TYR:CD2	0.63	2.52	12	1
1:A:58:VAL:HG12	1:A:75:THR:CG2	0.62	2.24	12	2
1:A:24:ALA:HB1	1:A:57:ALA:CB	0.62	2.24	8	4
1:A:58:VAL:HG12	1:A:75:THR:HG22	0.61	1.71	12	1
1:A:101:ILE:HG23	1:A:109:LYS:HD3	0.60	1.73	3	1
1:A:69:ILE:CG2	1:A:86:VAL:HG22	0.60	2.26	14	3
1:A:32:LEU:HD12	1:A:34:PHE:CE2	0.59	2.32	12	4
1:A:24:ALA:HB1	1:A:57:ALA:HA	0.59	1.73	5	3
1:A:100:LEU:CD2	1:A:114:LEU:HD11	0.59	2.26	10	1
1:A:34:PHE:CE1	1:A:43:THR:HG22	0.59	2.32	16	3
1:A:54:ASN:O	1:A:78:VAL:HG21	0.58	1.99	6	4
1:A:48:LEU:HD22	1:A:82:MET:O	0.58	1.97	11	5
1:A:89:GLU:N	1:A:89:GLU:CD	0.57	2.58	12	2
1:A:34:PHE:CE1	1:A:45:LYS:HD2	0.57	2.35	12	1
1:A:49:VAL:HG21	1:A:84:LEU:HD12	0.56	1.77	7	1
1:A:34:PHE:CE1	1:A:45:LYS:HD3	0.56	2.35	12	6
1:A:39:VAL:HG12	1:A:119:ILE:O	0.56	2.01	9	3
1:A:39:VAL:CG2	1:A:90:PRO:O	0.55	2.54	20	1
1:A:50:ARG:NH1	1:A:52:ILE:CG2	0.55	2.69	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:VAL:HG13	1:A:40:LYS:N	0.55	2.17	11	14
1:A:26:LEU:HD13	1:A:51:ASN:HA	0.55	1.79	5	5
1:A:26:LEU:HD23	1:A:104:TYR:HE1	0.55	1.61	7	3
1:A:32:LEU:HD11	1:A:45:LYS:HE3	0.55	1.78	2	3
1:A:25:ILE:C	1:A:26:LEU:HD22	0.54	2.23	8	6
1:A:26:LEU:CD2	1:A:57:ALA:HB1	0.54	2.30	5	3
1:A:32:LEU:CD1	1:A:34:PHE:CE2	0.54	2.90	12	2
1:A:54:ASN:C	1:A:78:VAL:HG21	0.54	2.24	6	1
1:A:51:ASN:CB	1:A:77:ASN:O	0.54	2.56	16	2
1:A:39:VAL:HG11	1:A:93:VAL:CG2	0.53	2.33	19	1
1:A:25:ILE:HG22	1:A:52:ILE:HD11	0.53	1.78	1	2
1:A:39:VAL:HB	1:A:118:ALA:HB1	0.53	1.79	6	1
1:A:109:LYS:CE	1:A:111:PHE:CZ	0.53	2.91	12	2
1:A:81:SER:OG	1:A:82:MET:N	0.53	2.42	15	1
1:A:60:HIS:CG	1:A:73:ILE:HD12	0.53	2.39	20	2
1:A:101:ILE:HG21	1:A:109:LYS:HE2	0.52	1.81	19	1
1:A:54:ASN:ND2	1:A:55:LYS:N	0.52	2.57	11	1
1:A:65:ARG:HA	1:A:67:PHE:N	0.52	2.19	4	19
1:A:69:ILE:HG21	1:A:86:VAL:HG22	0.52	1.80	14	1
1:A:109:LYS:HE3	1:A:111:PHE:CZ	0.52	2.39	12	2
1:A:34:PHE:CD2	1:A:43:THR:HG21	0.52	2.39	18	1
1:A:54:ASN:O	1:A:78:VAL:HG11	0.52	2.05	16	2
1:A:67:PHE:CE2	1:A:88:PHE:CD1	0.52	2.97	12	1
1:A:24:ALA:C	1:A:25:ILE:HD13	0.52	2.23	13	1
1:A:31:LYS:HA	1:A:112:VAL:HG13	0.51	1.82	6	1
1:A:34:PHE:CZ	1:A:45:LYS:HB2	0.51	2.40	16	1
1:A:39:VAL:CG1	1:A:93:VAL:HG22	0.51	2.34	19	1
1:A:46:ILE:HG21	1:A:83:GLN:CD	0.51	2.26	3	2
1:A:76:LEU:HD13	1:A:82:MET:HB3	0.51	1.81	11	2
1:A:34:PHE:CE1	1:A:45:LYS:HB2	0.51	2.41	16	3
1:A:51:ASN:OD1	1:A:78:VAL:HG22	0.51	2.06	1	2
1:A:32:LEU:CD2	1:A:34:PHE:CE2	0.51	2.93	16	1
1:A:34:PHE:CE1	1:A:43:THR:CG2	0.51	2.94	2	2
1:A:101:ILE:HG12	1:A:111:PHE:CE2	0.51	2.41	10	7
1:A:88:PHE:CD1	1:A:88:PHE:O	0.50	2.64	18	1
1:A:39:VAL:CG2	1:A:91:GLN:O	0.50	2.59	20	2
1:A:106:THR:HG23	1:A:107:GLY:N	0.50	2.21	6	4
1:A:32:LEU:C	1:A:32:LEU:CD1	0.50	2.80	4	2
1:A:48:LEU:C	1:A:48:LEU:HD13	0.50	2.27	9	4
1:A:58:VAL:HG21	1:A:105:ASP:CB	0.50	2.35	18	1
1:A:26:LEU:CD2	1:A:57:ALA:CB	0.50	2.89	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:PHE:CE2	1:A:45:LYS:HB2	0.50	2.41	9	1
1:A:59:PHE:CE1	1:A:74:GLY:O	0.50	2.65	12	1
1:A:32:LEU:CD1	1:A:34:PHE:CD2	0.50	2.94	7	6
1:A:60:HIS:ND1	1:A:73:ILE:HD12	0.50	2.22	3	1
1:A:34:PHE:CE2	1:A:45:LYS:HD3	0.50	2.42	17	3
1:A:32:LEU:HD22	1:A:34:PHE:CD1	0.49	2.42	17	2
1:A:32:LEU:C	1:A:32:LEU:HD13	0.49	2.28	4	3
1:A:89:GLU:OE1	1:A:91:GLN:NE2	0.49	2.46	1	1
1:A:93:VAL:HG13	1:A:119:ILE:C	0.49	2.27	16	1
1:A:34:PHE:CE1	1:A:45:LYS:HE2	0.49	2.42	14	2
1:A:58:VAL:HG22	1:A:105:ASP:N	0.49	2.23	7	1
1:A:50:ARG:NH1	1:A:52:ILE:HG23	0.49	2.22	20	1
1:A:43:THR:C	1:A:44:GLN:NE2	0.48	2.67	16	3
1:A:48:LEU:HD13	1:A:48:LEU:C	0.48	2.28	18	4
1:A:59:PHE:CD1	1:A:74:GLY:O	0.48	2.66	12	1
1:A:69:ILE:CG2	1:A:86:VAL:HG13	0.48	2.37	1	1
1:A:39:VAL:O	1:A:90:PRO:O	0.48	2.31	20	15
1:A:101:ILE:HD12	1:A:111:PHE:CE1	0.48	2.43	12	2
1:A:64:CYS:C	1:A:67:PHE:O	0.48	2.52	9	9
1:A:32:LEU:HD11	1:A:45:LYS:CD	0.48	2.37	14	1
1:A:58:VAL:HG22	1:A:75:THR:CG2	0.48	2.38	19	1
1:A:46:ILE:CD1	1:A:85:GLU:OE2	0.48	2.62	13	1
1:A:68:SER:O	1:A:87:GLU:N	0.48	2.47	20	3
1:A:34:PHE:CD2	1:A:45:LYS:HD3	0.48	2.43	5	1
1:A:70:GLU:HA	1:A:71:PRO:C	0.47	2.30	18	20
1:A:67:PHE:CZ	1:A:114:LEU:HB3	0.47	2.44	3	2
1:A:49:VAL:CG2	1:A:84:LEU:HD12	0.47	2.39	7	1
1:A:67:PHE:CD1	1:A:88:PHE:CD1	0.47	3.02	20	3
1:A:34:PHE:O	1:A:35:SER:C	0.47	2.53	18	1
1:A:60:HIS:HB3	1:A:103:CYS:SG	0.47	2.49	3	1
1:A:67:PHE:CG	1:A:114:LEU:HD13	0.47	2.44	6	2
1:A:34:PHE:CE1	1:A:45:LYS:HE3	0.47	2.44	4	1
1:A:99:ARG:HD2	1:A:111:PHE:CD1	0.47	2.43	15	1
1:A:60:HIS:CD2	1:A:73:ILE:HB	0.47	2.45	7	3
1:A:93:VAL:HG11	1:A:120:ASP:OD1	0.47	2.10	4	1
1:A:58:VAL:HG22	1:A:105:ASP:CB	0.47	2.40	7	1
1:A:65:ARG:HB2	1:A:66:PRO:HA	0.47	1.87	10	2
1:A:26:LEU:HD23	1:A:104:TYR:OH	0.47	2.09	12	1
1:A:39:VAL:CG1	1:A:119:ILE:O	0.47	2.63	18	2
1:A:28:PHE:CD2	1:A:47:LEU:HD21	0.47	2.45	7	3
1:A:60:HIS:C	1:A:60:HIS:CD2	0.47	2.89	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD21	1:A:45:LYS:NZ	0.47	2.24	17	1
1:A:58:VAL:CB	1:A:75:THR:HG22	0.46	2.39	7	1
1:A:34:PHE:CD1	1:A:45:LYS:HD2	0.46	2.46	12	1
1:A:109:LYS:HE2	1:A:111:PHE:CZ	0.46	2.45	4	2
1:A:34:PHE:CD1	1:A:43:THR:HG21	0.46	2.46	2	1
1:A:91:GLN:NE2	1:A:91:GLN:HA	0.46	2.25	8	4
1:A:34:PHE:CE2	1:A:45:LYS:HE2	0.46	2.46	9	1
1:A:61:ILE:O	1:A:72:ALA:HB1	0.46	2.09	14	1
1:A:26:LEU:HD23	1:A:104:TYR:CE1	0.46	2.44	7	1
1:A:26:LEU:HD21	1:A:57:ALA:HB3	0.46	1.83	9	2
1:A:38:PRO:CG	1:A:41:TYR:HB2	0.46	2.41	13	18
1:A:101:ILE:HG12	1:A:111:PHE:CD2	0.46	2.45	8	3
1:A:46:ILE:HG21	1:A:83:GLN:NE2	0.46	2.25	3	1
1:A:88:PHE:CE2	1:A:90:PRO:HD3	0.46	2.46	17	2
1:A:34:PHE:CD2	1:A:45:LYS:HE2	0.45	2.45	9	1
1:A:120:ASP:O	1:A:120:ASP:CG	0.45	2.55	1	2
1:A:34:PHE:CD1	1:A:45:LYS:HE3	0.45	2.46	4	1
1:A:65:ARG:HA	1:A:66:PRO:C	0.45	2.32	7	20
1:A:119:ILE:HD12	1:A:119:ILE:O	0.45	2.11	5	1
1:A:104:TYR:CD2	1:A:108:GLU:HB2	0.45	2.46	13	1
1:A:56:ASN:O	1:A:56:ASN:CG	0.45	2.55	5	1
1:A:51:ASN:C	1:A:51:ASN:OD1	0.45	2.55	6	2
1:A:34:PHE:CE1	1:A:45:LYS:CE	0.45	3.00	7	1
1:A:50:ARG:NH1	1:A:79:GLY:O	0.45	2.50	15	1
1:A:88:PHE:CE2	1:A:116:GLY:HA3	0.45	2.47	7	1
1:A:68:SER:C	1:A:69:ILE:CG2	0.44	2.85	3	1
1:A:58:VAL:CG2	1:A:105:ASP:HB2	0.44	2.42	7	1
1:A:25:ILE:O	1:A:26:LEU:HD22	0.44	2.11	9	2
1:A:25:ILE:CG2	1:A:52:ILE:HD11	0.44	2.42	19	1
1:A:100:LEU:HG	1:A:114:LEU:HD21	0.44	1.89	15	1
1:A:61:ILE:N	1:A:72:ALA:O	0.44	2.50	14	2
1:A:48:LEU:C	1:A:48:LEU:CD1	0.44	2.86	18	3
1:A:88:PHE:O	1:A:88:PHE:CD2	0.44	2.70	7	2
1:A:64:CYS:O	1:A:67:PHE:O	0.44	2.36	18	10
1:A:34:PHE:CD1	1:A:45:LYS:CD	0.44	3.01	12	1
1:A:110:VAL:HG12	1:A:111:PHE:N	0.44	2.28	12	3
1:A:46:ILE:HG21	1:A:83:GLN:HE21	0.44	1.72	11	1
1:A:39:VAL:CG2	1:A:91:GLN:C	0.44	2.86	20	1
1:A:67:PHE:CE1	1:A:88:PHE:CG	0.44	3.06	6	2
1:A:76:LEU:HD13	1:A:82:MET:CG	0.43	2.43	10	1
1:A:109:LYS:HD2	1:A:111:PHE:CZ	0.43	2.48	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:PHE:CD1	1:A:115:TYR:O	0.43	2.72	19	1
1:A:69:ILE:O	1:A:69:ILE:HD13	0.43	2.13	13	2
1:A:68:SER:O	1:A:69:ILE:HG22	0.43	2.14	3	1
1:A:59:PHE:HB2	1:A:102:VAL:CG1	0.43	2.43	18	2
1:A:60:HIS:CD2	1:A:60:HIS:C	0.43	2.93	10	1
1:A:39:VAL:HG22	1:A:40:LYS:N	0.43	2.27	15	1
1:A:68:SER:O	1:A:87:GLU:O	0.43	2.37	16	6
1:A:25:ILE:HG22	1:A:26:LEU:N	0.42	2.29	9	1
1:A:40:LYS:CD	1:A:91:GLN:NE2	0.42	2.81	20	1
1:A:51:ASN:OD1	1:A:51:ASN:C	0.42	2.58	1	1
1:A:90:PRO:CG	1:A:118:ALA:HB2	0.42	2.44	18	2
1:A:39:VAL:HG13	1:A:40:LYS:HD3	0.42	1.91	6	1
1:A:93:VAL:HG23	1:A:119:ILE:CA	0.42	2.43	18	1
1:A:77:ASN:OD1	1:A:77:ASN:N	0.42	2.52	3	2
1:A:82:MET:SD	1:A:83:GLN:O	0.42	2.78	13	4
1:A:61:ILE:CG1	1:A:102:VAL:HG13	0.42	2.45	12	1
1:A:67:PHE:CD1	1:A:88:PHE:HB2	0.42	2.49	8	2
1:A:54:ASN:OD1	1:A:54:ASN:N	0.42	2.52	6	1
1:A:43:THR:CG2	1:A:44:GLN:N	0.42	2.83	18	1
1:A:93:VAL:HG23	1:A:119:ILE:C	0.42	2.35	18	1
1:A:89:GLU:N	1:A:89:GLU:OE1	0.42	2.52	12	1
1:A:69:ILE:HD13	1:A:69:ILE:O	0.42	2.15	17	1
1:A:99:ARG:HD3	1:A:111:PHE:CD1	0.41	2.50	11	1
1:A:40:LYS:O	1:A:89:GLU:OE2	0.41	2.38	13	1
1:A:49:VAL:O	1:A:76:LEU:HD21	0.41	2.15	15	1
1:A:90:PRO:O	1:A:91:GLN:C	0.41	2.58	18	1
1:A:24:ALA:HB1	1:A:57:ALA:CA	0.41	2.45	9	1
1:A:51:ASN:HB3	1:A:77:ASN:O	0.41	2.15	20	1
1:A:44:GLN:NE2	1:A:87:GLU:HG3	0.41	2.30	15	1
1:A:55:LYS:HD2	1:A:56:ASN:N	0.41	2.30	16	1
1:A:70:GLU:HG3	1:A:71:PRO:N	0.41	2.30	8	1
1:A:60:HIS:CG	1:A:73:ILE:HB	0.41	2.51	15	1
1:A:32:LEU:CD1	1:A:34:PHE:CE1	0.41	2.99	8	1
1:A:27:ASP:OD1	1:A:27:ASP:C	0.41	2.60	3	1
1:A:88:PHE:CZ	1:A:90:PRO:HD3	0.41	2.51	12	1
1:A:32:LEU:HD13	1:A:32:LEU:C	0.41	2.36	2	1
1:A:25:ILE:N	1:A:25:ILE:HD13	0.41	2.31	6	1
1:A:26:LEU:HD23	1:A:104:TYR:HE2	0.41	1.75	15	1
1:A:101:ILE:HG23	1:A:109:LYS:CD	0.40	2.44	3	1
1:A:39:VAL:HG23	1:A:92:SER:C	0.40	2.36	18	1
1:A:65:ARG:HB3	1:A:65:ARG:CZ	0.40	2.47	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD11	1:A:81:SER:HB3	0.40	1.93	17	1
1:A:54:ASN:CG	1:A:55:LYS:N	0.40	2.73	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	97/122 (80%)	88±2 (91±2%)	6±2 (7±2%)	3±1 (3±1%)	8	44
All	All	1940/2440 (80%)	1761 (91%)	128 (7%)	51 (3%)	8	44

All 6 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	116	GLY	20
1	A	35	SER	18
1	A	117	ALA	7
1	A	107	GLY	4
1	A	53	GLY	1
1	A	41	TYR	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	85/104 (82%)	79±2 (93±3%)	6±2 (7±3%)	17	65
All	All	1700/2080 (82%)	1573 (93%)	127 (7%)	17	65

All 31 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	69	ILE	20
1	A	32	LEU	14
1	A	95	ASP	9
1	A	120	ASP	8
1	A	70	GLU	7
1	A	91	GLN	5
1	A	54	ASN	5
1	A	62	LYS	5
1	A	31	LYS	5
1	A	40	LYS	5
1	A	48	LEU	5
1	A	77	ASN	4
1	A	39	VAL	3
1	A	30	ASP	3
1	A	55	LYS	3
1	A	68	SER	3
1	A	105	ASP	3
1	A	50	ARG	3
1	A	113	SER	2
1	A	89	GLU	2
1	A	56	ASN	2
1	A	27	ASP	2
1	A	58	VAL	1
1	A	45	LYS	1
1	A	106	THR	1
1	A	99	ARG	1
1	A	108	GLU	1
1	A	85	GLU	1
1	A	110	VAL	1
1	A	81	SER	1
1	A	88	PHE	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