Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 02:31 PM EST

PDB ID	:	2DAY
Title	:	Solution structure of the RWD domain of human ring finger protein 25
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Deposited on	:	2005-12-14

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:

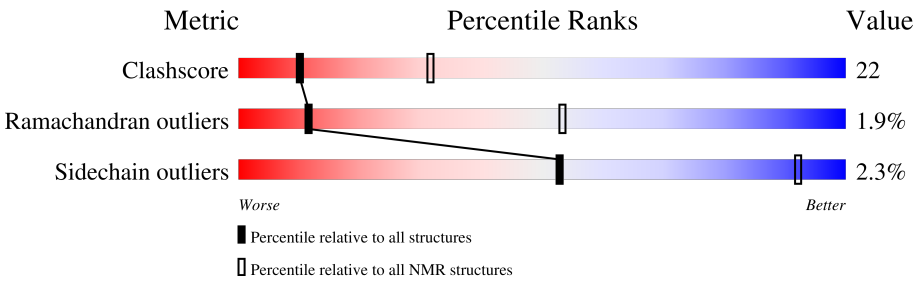
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	128	46% 27% 27%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 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:11-A:31, A:40-A:47, A:59-A:122 (93)	0.22	18

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1949 atoms, of which 966 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RING finger protein 25.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	128	1949	622	966	160	199	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q96BH1
A	2	SER	-	cloning artifact	UNP Q96BH1
A	3	SER	-	cloning artifact	UNP Q96BH1
A	4	GLY	-	cloning artifact	UNP Q96BH1
A	5	SER	-	cloning artifact	UNP Q96BH1
A	6	SER	-	cloning artifact	UNP Q96BH1
A	7	GLY	-	cloning artifact	UNP Q96BH1
A	123	SER	-	cloning artifact	UNP Q96BH1
A	124	GLY	-	cloning artifact	UNP Q96BH1
A	125	PRO	-	cloning artifact	UNP Q96BH1
A	126	SER	-	cloning artifact	UNP Q96BH1
A	127	SER	-	cloning artifact	UNP Q96BH1
A	128	GLY	-	cloning artifact	UNP Q96BH1

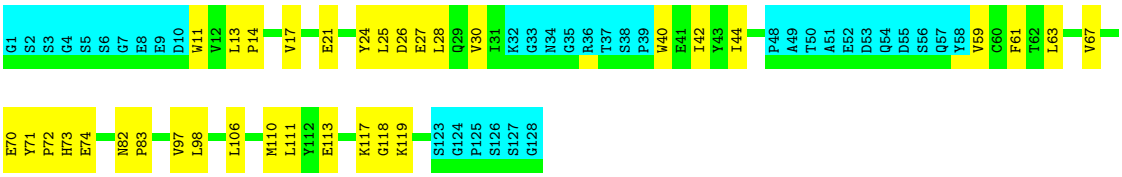
4 Residue-property plots (i)

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: RING finger protein 25

Chain A: 46% 27% 27%



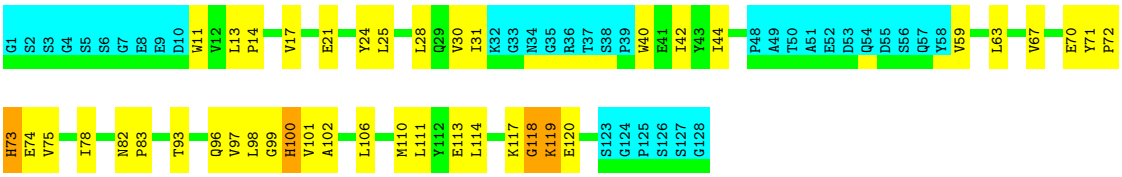
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: RING finger protein 25

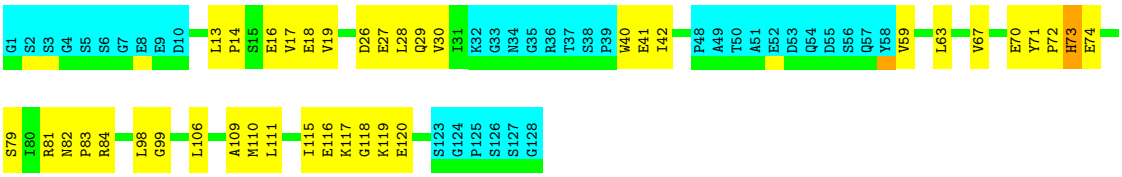
Chain A: 40% 30% • 27%



4.2.2 Score per residue for model 2

• Molecule 1: RING finger protein 25

Chain A: 42% 30% • 27%



4.2.3 Score per residue for model 3

- Molecule 1: RING finger protein 25

Chain A: 52% 20% • 27%

4.2.4 Score per residue for model 4

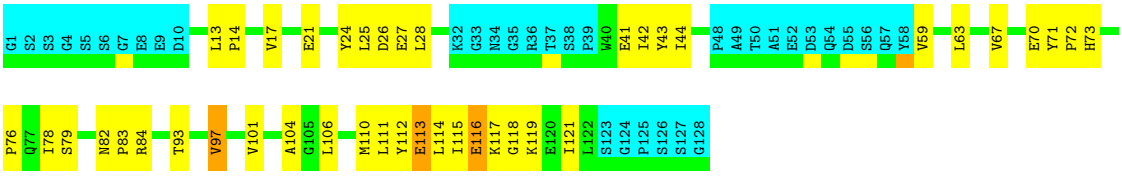
- Molecule 1: RING finger protein 25

Chain A: 41% 28% • 27%

4.2.5 Score per residue for model 5

- Molecule 1: RING finger protein 25

Chain A: 40% 30% • 27%



4.2.6 Score per residue for model 6

- Molecule 1: RING finger protein 25

Chain A: 44% 27% • 27%

G1 S2 S3 G4 S5 S6 G7 E8 E9 D10 W11 V12 L13 P14 S15 E16 V17 E18 V19 L20 E21 Y24 L25 V30 I31 K32 G33 N34 G35 R36 T37 S38 P39 W40 I44 P48 A49 T50 A51 E52 D53 Q54 D55 S56 Q57 Y58 V59 C60 F61 T62 L63 V67 E70 Y71

P72 H73 E74 N82 P83 Q90 I91 V97 L98 G99 H100 A104 G105 L106 M110 L111 K117 G118 K119 E120 I121 L122 S123 G124 P125 S126 S127 G128

4.2.7 Score per residue for model 7

- Molecule 1: RING finger protein 25

Chain A: 47% 25% • 27%

G1 S2 S3 G4 S5 S6 G7 E8 E9 D10 W11 V12 L13 P14 S15 E16 V17 E18 V19 L20 E21 L25 L28 Q29 V30 I31 K32 G33 N34 G35 R36 T37 S38 P39 W40 E41 I42 Y43 I44 P48 A49 T50 A51 E52 D53 Q54 D55 S56 Q57 Y58 V59 C60 F61 T62 L63 E70

Y71 P72 H73 I80 R81 N82 P83 I91 I94 L106 M110 L111 Y112 E113 L114 K117 G118 I121 L122 S123 G124 P125 S126 S127 G128

4.2.8 Score per residue for model 8

- Molecule 1: RING finger protein 25

Chain A: 46% 25% • 27%

G1 S2 S3 G4 S5 S6 G7 E8 E9 D10 W11 V12 L13 P14 V17 D26 E27 L28 Q29 V30 I31 K32 G33 N34 G35 R36 T37 S38 P39 W40 E41 I42 Y43 P48 A49 T50 A51 E52 D53 Q54 D55 S56 Q57 Y58 V59 V67 E70 Y71 P72 H73 E74 V75 N82 P83

S87 D88 T93 V97 A102 L106 M110 L111 Y112 E113 L114 E120 S123 G124 P125 S126 S127 G128

4.2.9 Score per residue for model 9

- Molecule 1: RING finger protein 25

Chain A: 42% 28% • • 27%

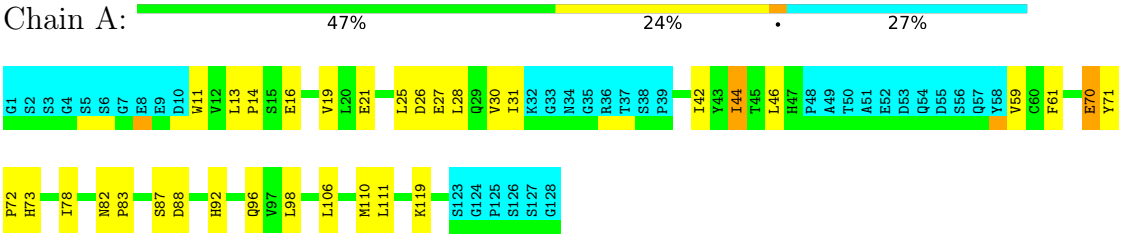
G1 S2 S3 G4 S5 S6 G7 E8 E9 D10 W11 V12 L13 P14 V17 E21 Y24 L25 V30 I31 K32 G33 N34 G35 R36 T37 S38 P39 W40 E41 I42 Y43 I44 T45 L46 H47 P48 A49 T50 A51 E52 D53 Q54 D55 S56 Q57 Y58 F61 T62 L63 V64 L65 Q66 V67

E70 Y71 P72 H73 E74 I80 R81 N82 P83 I91 L106 M110 L111 Y112 E113 L114 K117 G118 K119 E120 I121 L122 S123 G124 P125 S126 S127 G128

4.2.10 Score per residue for model 10

- Molecule 1: RING finger protein 25

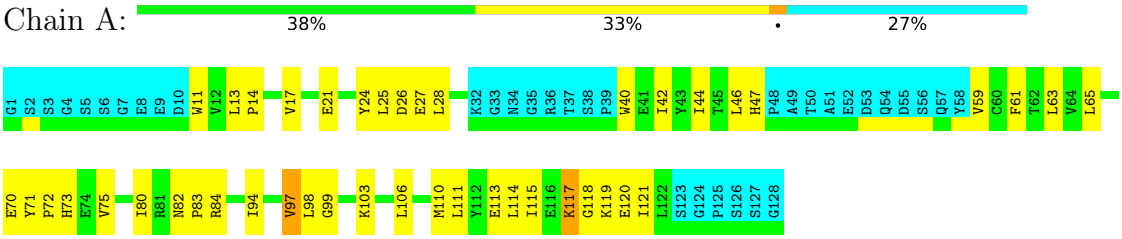
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: RING finger protein 25

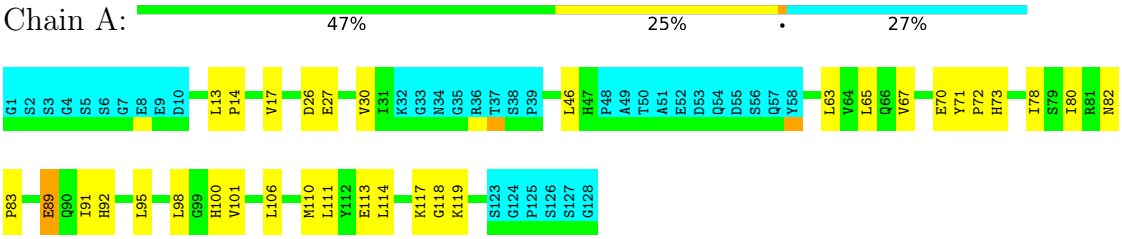
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: RING finger protein 25

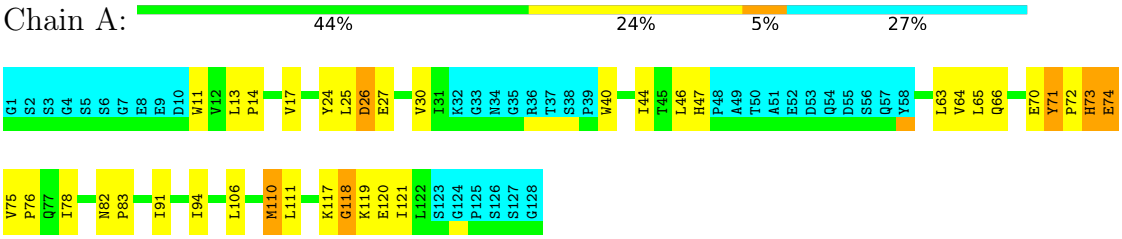
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: RING finger protein 25

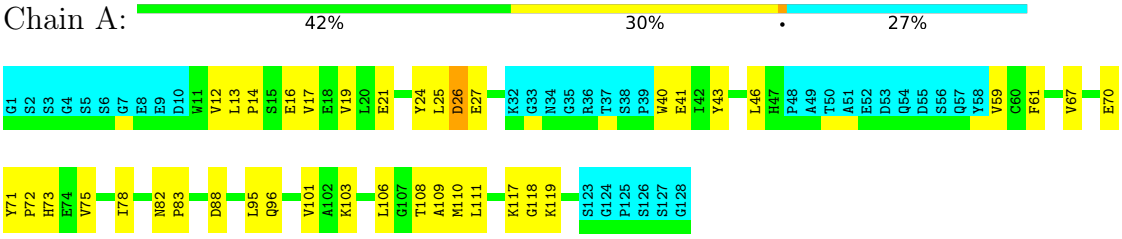
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: RING finger protein 25

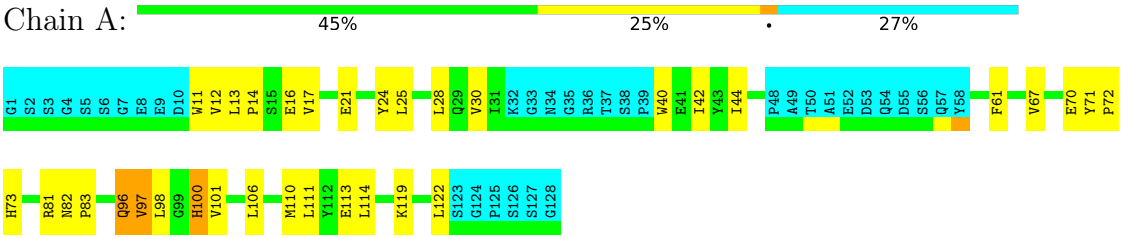
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: RING finger protein 25

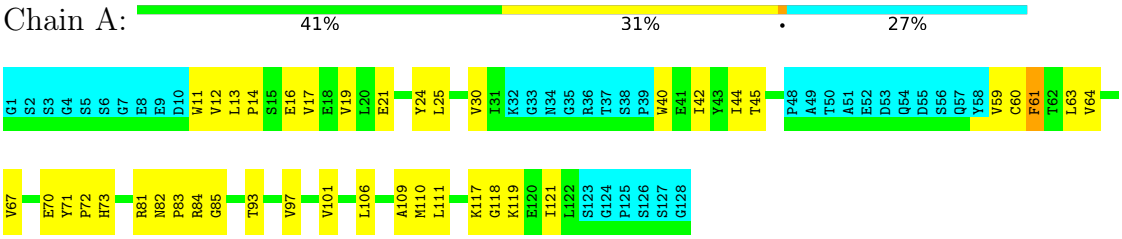
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: RING finger protein 25

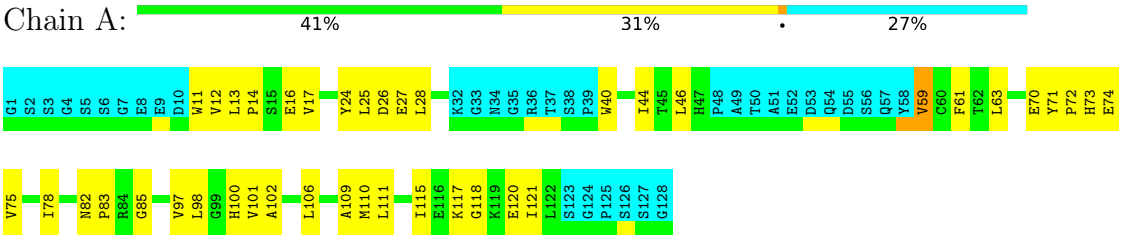
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: RING finger protein 25

Chain A:



4.2.18 Score per residue for model 18 (medoid)

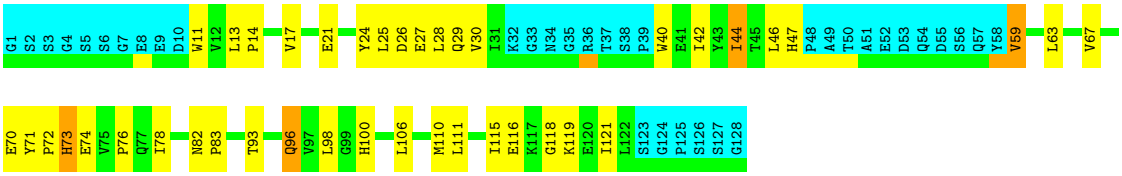
- Molecule 1: RING finger protein 25

Chain A: 41% 30% • 27%

4.2.19 Score per residue for model 19

- Molecule 1: RING finger protein 25

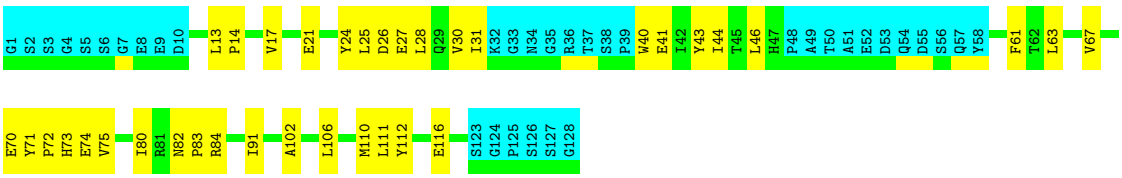
Chain A: 41% 29% • 27%



4.2.20 Score per residue for model 20

- Molecule 1: RING finger protein 25

Chain A: 45% 28% 27%



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: *target function,structures with the lowest energy,structures with the least restraint violations*.

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	747	768	764	33±6
All	All	14940	15360	15280	654

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD13	1:A:29:GLN:N	0.95	1.75	4	1
1:A:65:LEU:HD21	1:A:111:LEU:HD22	0.85	1.48	11	1
1:A:17:VAL:CG1	1:A:30:VAL:HG21	0.80	2.06	4	5
1:A:46:LEU:HD11	1:A:119:LYS:HG3	0.79	1.55	14	3
1:A:67:VAL:HG13	1:A:71:TYR:CD2	0.78	2.12	2	12
1:A:78:ILE:HD13	1:A:98:LEU:HB3	0.78	1.56	1	1
1:A:13:LEU:O	1:A:17:VAL:HG23	0.75	1.80	20	16
1:A:17:VAL:HG11	1:A:30:VAL:HG11	0.73	1.60	20	4
1:A:16:GLU:O	1:A:19:VAL:HG12	0.73	1.83	14	4
1:A:46:LEU:HD22	1:A:119:LYS:HG2	0.73	1.60	11	1
1:A:16:GLU:CD	1:A:109:ALA:HB2	0.71	2.05	16	1
1:A:31:ILE:HD12	1:A:31:ILE:N	0.70	2.00	1	5
1:A:93:THR:O	1:A:97:VAL:HG23	0.70	1.85	8	3
1:A:63:LEU:HD22	1:A:65:LEU:CD2	0.70	2.16	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:HD11	1:A:43:TYR:CE2	0.70	2.22	4	2
1:A:17:VAL:HG13	1:A:30:VAL:HG21	0.68	1.64	20	9
1:A:11:TRP:CZ2	1:A:13:LEU:HD23	0.65	2.26	9	6
1:A:28:LEU:HB2	1:A:44:ILE:HD12	0.64	1.69	7	3
1:A:67:VAL:CG1	1:A:71:TYR:CG	0.64	2.80	2	7
1:A:63:LEU:HD22	1:A:65:LEU:HD11	0.64	1.69	13	1
1:A:118:GLY:HA2	1:A:121:ILE:HD12	0.63	1.68	17	5
1:A:100:HIS:CE1	1:A:104:ALA:HB2	0.63	2.29	6	1
1:A:28:LEU:HD11	1:A:42:ILE:HG21	0.62	1.72	7	8
1:A:17:VAL:HG11	1:A:30:VAL:HG21	0.61	1.71	4	1
1:A:80:ILE:HD12	1:A:91:ILE:HG23	0.60	1.73	9	4
1:A:92:HIS:CE1	1:A:96:GLN:NE2	0.60	2.68	10	1
1:A:75:VAL:HG11	1:A:103:LYS:HG3	0.60	1.71	11	1
1:A:46:LEU:HD21	1:A:119:LYS:N	0.60	2.11	10	1
1:A:29:GLN:O	1:A:42:ILE:HG23	0.60	1.97	2	3
1:A:78:ILE:HG21	1:A:98:LEU:HD13	0.60	1.73	17	1
1:A:11:TRP:CE2	1:A:13:LEU:HD23	0.59	2.32	9	4
1:A:30:VAL:HG22	1:A:42:ILE:HG12	0.59	1.73	16	4
1:A:13:LEU:HD21	1:A:40:TRP:CG	0.59	2.33	2	11
1:A:61:PHE:CD2	1:A:80:ILE:HG23	0.59	2.33	11	1
1:A:75:VAL:HG11	1:A:103:LYS:CG	0.58	2.28	11	1
1:A:71:TYR:C	1:A:71:TYR:CD1	0.58	2.77	9	12
1:A:31:ILE:N	1:A:31:ILE:CD1	0.58	2.67	1	2
1:A:13:LEU:HD13	1:A:67:VAL:HG11	0.58	1.75	8	4
1:A:46:LEU:HD22	1:A:119:LYS:CG	0.58	2.29	11	2
1:A:28:LEU:HD11	1:A:42:ILE:CG2	0.57	2.28	11	5
1:A:28:LEU:C	1:A:28:LEU:HD23	0.57	2.20	11	6
1:A:112:TYR:CD1	1:A:116:GLU:OE2	0.57	2.58	5	1
1:A:13:LEU:HD21	1:A:40:TRP:CD2	0.57	2.34	9	3
1:A:31:ILE:CD1	1:A:43:TYR:CE2	0.57	2.88	4	2
1:A:75:VAL:HB	1:A:102:ALA:HB1	0.57	1.75	8	4
1:A:82:ASN:N	1:A:83:PRO:CD	0.56	2.67	2	20
1:A:78:ILE:HG21	1:A:98:LEU:CD1	0.56	2.30	17	3
1:A:67:VAL:HG13	1:A:71:TYR:CG	0.56	2.34	16	5
1:A:97:VAL:HG13	1:A:98:LEU:N	0.56	2.15	18	2
1:A:17:VAL:HA	1:A:20:LEU:HD12	0.56	1.77	3	2
1:A:59:VAL:HG23	1:A:85:GLY:HA3	0.56	1.78	16	4
1:A:111:LEU:O	1:A:115:ILE:HD12	0.55	2.00	11	2
1:A:61:PHE:CE2	1:A:122:LEU:HD11	0.55	2.37	15	1
1:A:63:LEU:C	1:A:63:LEU:HD23	0.54	2.22	11	1
1:A:67:VAL:CG1	1:A:71:TYR:CD2	0.54	2.89	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TRP:CZ2	1:A:13:LEU:CD2	0.54	2.91	19	3
1:A:63:LEU:HD11	1:A:98:LEU:HD13	0.53	1.81	2	1
1:A:63:LEU:HD22	1:A:65:LEU:CD1	0.53	2.32	13	1
1:A:61:PHE:C	1:A:61:PHE:CD1	0.53	2.81	17	7
1:A:46:LEU:HD22	1:A:119:LYS:HG3	0.53	1.80	19	2
1:A:100:HIS:CG	1:A:101:VAL:N	0.53	2.77	17	3
1:A:28:LEU:HD13	1:A:28:LEU:C	0.53	2.23	4	1
1:A:94:ILE:HG23	1:A:121:ILE:HG21	0.53	1.78	11	3
1:A:31:ILE:HD11	1:A:43:TYR:CD2	0.52	2.38	4	1
1:A:112:TYR:CE2	1:A:116:GLU:CD	0.52	2.83	20	1
1:A:16:GLU:CD	1:A:109:ALA:HB1	0.52	2.25	17	2
1:A:65:LEU:HD21	1:A:111:LEU:CD2	0.52	2.28	11	1
1:A:46:LEU:HD21	1:A:118:GLY:C	0.51	2.26	12	2
1:A:75:VAL:HG13	1:A:106:LEU:HD11	0.51	1.82	14	1
1:A:78:ILE:HD13	1:A:98:LEU:CB	0.51	2.32	1	2
1:A:28:LEU:CD1	1:A:30:VAL:HG23	0.51	2.35	4	1
1:A:61:PHE:HD2	1:A:80:ILE:HG23	0.51	1.63	11	1
1:A:70:GLU:O	1:A:71:TYR:C	0.51	2.49	8	20
1:A:64:VAL:HG12	1:A:66:GLN:OE1	0.51	2.06	13	1
1:A:72:PRO:O	1:A:73:HIS:C	0.51	2.48	9	20
1:A:72:PRO:O	1:A:106:LEU:CD2	0.50	2.60	6	20
1:A:97:VAL:HG13	1:A:98:LEU:H	0.50	1.66	1	1
1:A:11:TRP:NE1	1:A:71:TYR:O	0.50	2.45	8	5
1:A:96:GLN:OE1	1:A:97:VAL:N	0.49	2.45	15	1
1:A:44:ILE:HG23	1:A:63:LEU:HB3	0.49	1.83	19	1
1:A:76:PRO:O	1:A:78:ILE:HD12	0.49	2.08	13	4
1:A:94:ILE:HG23	1:A:121:ILE:HD13	0.49	1.84	11	1
1:A:45:THR:CG2	1:A:60:CYS:SG	0.49	3.00	16	1
1:A:21:GLU:O	1:A:25:LEU:N	0.49	2.45	16	14
1:A:63:LEU:HD22	1:A:65:LEU:HD22	0.49	1.83	12	1
1:A:117:LYS:O	1:A:120:GLU:N	0.49	2.46	6	2
1:A:13:LEU:HB2	1:A:71:TYR:CD1	0.48	2.43	8	5
1:A:46:LEU:C	1:A:47:HIS:CD2	0.48	2.87	13	1
1:A:92:HIS:NE2	1:A:96:GLN:NE2	0.48	2.61	10	1
1:A:28:LEU:HD22	1:A:43:TYR:O	0.48	2.09	4	1
1:A:71:TYR:CG	1:A:72:PRO:HA	0.48	2.43	9	20
1:A:93:THR:O	1:A:97:VAL:HG12	0.47	2.09	1	2
1:A:26:ASP:O	1:A:28:LEU:N	0.47	2.47	4	1
1:A:44:ILE:HG22	1:A:63:LEU:HB3	0.47	1.86	17	3
1:A:72:PRO:O	1:A:74:GLU:N	0.47	2.47	9	9
1:A:13:LEU:HB2	1:A:71:TYR:CE1	0.47	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:TYR:HA	1:A:72:PRO:C	0.47	2.30	8	20
1:A:13:LEU:N	1:A:14:PRO:HD2	0.47	2.24	15	20
1:A:78:ILE:HG21	1:A:98:LEU:HD12	0.47	1.85	19	1
1:A:41:GLU:HG2	1:A:43:TYR:CE1	0.47	2.45	8	3
1:A:14:PRO:HB3	1:A:40:TRP:CH2	0.46	2.46	9	12
1:A:46:LEU:CB	1:A:61:PHE:CE2	0.46	2.98	20	1
1:A:61:PHE:CE2	1:A:122:LEU:HD21	0.46	2.46	9	1
1:A:81:ARG:O	1:A:82:ASN:C	0.46	2.54	16	3
1:A:101:VAL:HG21	1:A:117:LYS:HG3	0.46	1.88	16	2
1:A:13:LEU:CB	1:A:14:PRO:CD	0.46	2.94	7	20
1:A:31:ILE:HD13	1:A:43:TYR:CE2	0.46	2.46	20	1
1:A:41:GLU:OE1	1:A:66:GLN:CD	0.45	2.55	9	1
1:A:89:GLU:OE1	1:A:89:GLU:C	0.45	2.55	12	1
1:A:93:THR:HG23	1:A:96:GLN:NE2	0.45	2.26	19	1
1:A:24:TYR:O	1:A:25:LEU:C	0.45	2.55	16	15
1:A:117:LYS:O	1:A:118:GLY:C	0.45	2.55	2	14
1:A:110:MET:O	1:A:111:LEU:C	0.45	2.55	19	19
1:A:17:VAL:O	1:A:19:VAL:N	0.45	2.50	2	1
1:A:26:ASP:O	1:A:27:GLU:C	0.45	2.55	2	14
1:A:115:ILE:O	1:A:116:GLU:C	0.45	2.55	2	3
1:A:111:LEU:O	1:A:115:ILE:CD1	0.45	2.64	11	1
1:A:12:VAL:HG22	1:A:16:GLU:HG2	0.45	1.87	15	1
1:A:30:VAL:C	1:A:31:ILE:HD12	0.45	2.32	9	2
1:A:12:VAL:O	1:A:13:LEU:C	0.45	2.55	17	4
1:A:93:THR:O	1:A:97:VAL:CG2	0.45	2.62	16	1
1:A:71:TYR:CD1	1:A:72:PRO:N	0.45	2.85	9	10
1:A:116:GLU:N	1:A:116:GLU:OE1	0.45	2.50	5	1
1:A:28:LEU:HD21	1:A:30:VAL:CG2	0.44	2.42	1	1
1:A:11:TRP:CD1	1:A:13:LEU:HB3	0.44	2.46	13	3
1:A:28:LEU:HD11	1:A:30:VAL:HG23	0.44	1.89	4	1
1:A:16:GLU:O	1:A:19:VAL:CG1	0.44	2.63	14	1
1:A:78:ILE:HG22	1:A:95:LEU:CD2	0.44	2.42	14	1
1:A:74:GLU:CD	1:A:75:VAL:N	0.44	2.71	4	2
1:A:101:VAL:HG13	1:A:113:GLU:OE2	0.44	2.13	4	1
1:A:43:TYR:CD2	1:A:64:VAL:HG22	0.44	2.48	9	1
1:A:97:VAL:CG1	1:A:98:LEU:N	0.44	2.81	18	1
1:A:46:LEU:HG	1:A:61:PHE:CZ	0.44	2.48	20	1
1:A:98:LEU:O	1:A:99:GLY:C	0.44	2.56	11	4
1:A:87:SER:O	1:A:88:ASP:C	0.44	2.56	10	2
1:A:101:VAL:O	1:A:104:ALA:HB3	0.44	2.13	5	1
1:A:113:GLU:OE1	1:A:113:GLU:C	0.43	2.56	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:HG21	1:A:81:ARG:CG	0.43	2.42	16	1
1:A:76:PRO:CD	1:A:110:MET:SD	0.43	3.06	13	1
1:A:117:LYS:O	1:A:119:LYS:N	0.43	2.51	13	2
1:A:92:HIS:HA	1:A:95:LEU:HD12	0.43	1.90	12	1
1:A:118:GLY:O	1:A:119:LYS:C	0.43	2.56	5	2
1:A:40:TRP:N	1:A:67:VAL:O	0.43	2.51	9	1
1:A:20:LEU:O	1:A:23:ILE:N	0.43	2.51	4	2
1:A:113:GLU:O	1:A:114:LEU:C	0.43	2.58	11	9
1:A:30:VAL:HG23	1:A:42:ILE:HG13	0.43	1.91	7	1
1:A:61:PHE:CD1	1:A:61:PHE:C	0.43	2.91	15	2
1:A:71:TYR:CD2	1:A:72:PRO:HA	0.43	2.48	10	1
1:A:97:VAL:O	1:A:98:LEU:C	0.43	2.56	17	2
1:A:96:GLN:CG	1:A:97:VAL:N	0.42	2.83	1	1
1:A:59:VAL:HG23	1:A:84:ARG:O	0.42	2.14	11	1
1:A:70:GLU:CB	1:A:74:GLU:HB2	0.42	2.44	19	1
1:A:90:GLN:O	1:A:91:ILE:C	0.42	2.58	6	1
1:A:95:LEU:O	1:A:96:GLN:C	0.42	2.58	14	1
1:A:17:VAL:C	1:A:19:VAL:N	0.42	2.73	2	1
1:A:97:VAL:HG12	1:A:98:LEU:N	0.42	2.29	15	2
1:A:20:LEU:O	1:A:21:GLU:C	0.42	2.58	4	1
1:A:41:GLU:HG2	1:A:43:TYR:CZ	0.42	2.50	14	1
1:A:28:LEU:CD1	1:A:29:GLN:N	0.41	2.66	4	1
1:A:16:GLU:O	1:A:19:VAL:N	0.41	2.53	7	2
1:A:59:VAL:HG13	1:A:59:VAL:O	0.41	2.14	17	1
1:A:119:LYS:O	1:A:120:GLU:C	0.41	2.59	2	3
1:A:13:LEU:HD22	1:A:67:VAL:HG11	0.41	1.90	12	1
1:A:44:ILE:CG2	1:A:63:LEU:HB3	0.41	2.46	13	9
1:A:100:HIS:ND1	1:A:101:VAL:N	0.41	2.68	15	1
1:A:96:GLN:HG3	1:A:97:VAL:N	0.41	2.30	18	1
1:A:28:LEU:HD23	1:A:28:LEU:C	0.41	2.36	2	1
1:A:26:ASP:C	1:A:28:LEU:N	0.41	2.74	4	1
1:A:100:HIS:O	1:A:101:VAL:C	0.41	2.59	1	1
1:A:28:LEU:HD23	1:A:29:GLN:N	0.41	2.30	18	2
1:A:16:GLU:O	1:A:17:VAL:C	0.41	2.58	17	1
1:A:46:LEU:HD22	1:A:61:PHE:CZ	0.41	2.51	17	1
1:A:44:ILE:O	1:A:63:LEU:N	0.41	2.54	11	1
1:A:108:THR:O	1:A:109:ALA:C	0.41	2.59	14	1
1:A:78:ILE:H	1:A:78:ILE:HD12	0.41	1.75	17	1
1:A:118:GLY:O	1:A:121:ILE:N	0.40	2.54	5	1
1:A:103:LYS:HA	1:A:106:LEU:HD12	0.40	1.92	14	1
1:A:61:PHE:HE2	1:A:122:LEU:HD11	0.40	1.74	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ILE:O	1:A:44:ILE:HG23	0.40	2.16	10	1
1:A:70:GLU:HB2	1:A:74:GLU:CB	0.40	2.47	3	4
1:A:116:GLU:OE1	1:A:116:GLU:CA	0.40	2.69	5	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	93/128 (73%)	71±3 (77±3%)	20±3 (21±3%)	2±1 (2±1%)	11 53
All	All	1860/2560 (73%)	1427 (77%)	398 (21%)	35 (2%)	11 53

All 10 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	73	HIS	9
1	A	59	VAL	8
1	A	97	VAL	6
1	A	71	TYR	3
1	A	118	GLY	2
1	A	91	ILE	2
1	A	44	ILE	2
1	A	18	GLU	1
1	A	27	GLU	1
1	A	25	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	84/110 (76%)	82±1 (98±1%)	2±1 (2±1%)	53 92
All	All	1680/2200 (76%)	1641 (98%)	39 (2%)	53 92

All 23 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	100	HIS	4
1	A	88	ASP	3
1	A	120	GLU	3
1	A	26	ASP	3
1	A	119	LYS	2
1	A	79	SER	2
1	A	84	ARG	2
1	A	74	GLU	2
1	A	117	LYS	2
1	A	47	HIS	2
1	A	96	GLN	2
1	A	41	GLU	1
1	A	81	ARG	1
1	A	43	TYR	1
1	A	113	GLU	1
1	A	116	GLU	1
1	A	59	VAL	1
1	A	71	TYR	1
1	A	70	GLU	1
1	A	89	GLU	1
1	A	110	MET	1
1	A	61	PHE	1
1	A	28	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

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