



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:23 PM BST

PDB ID : 2JVB  
Title : Solution Structure of Catalytic Domain of yDcp2  
Authors : Deshmukh, M.; Gross, J.  
Deposited on : 2007-09-16

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

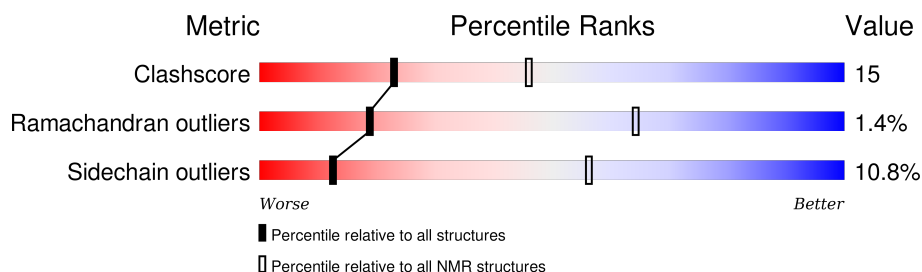
# 1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	146	 66% 29% . .

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:101-A:241 (141)	0.77	1

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 3 single-model clusters were found.

Cluster number	Models
1	4, 5, 7
2	1, 10
3	6, 9
Single-model clusters	2; 3; 8

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2446 atoms, of which 1225 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called mRNA-decapping enzyme subunit 2.

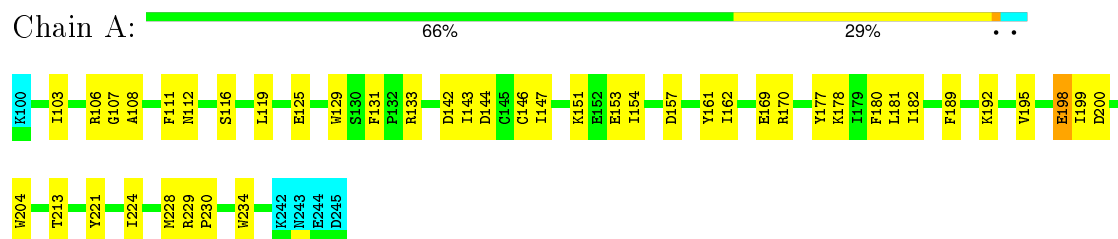
Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	0
			2446	780	1225	208	227	6	

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: mRNA-decapping enzyme subunit 2

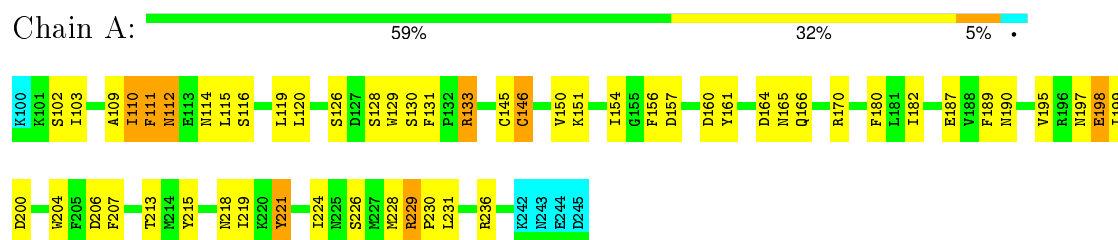


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

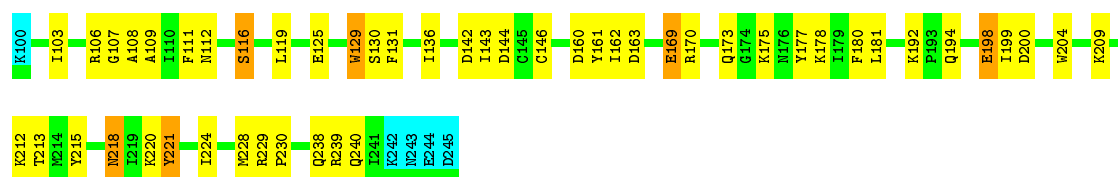
- Molecule 1: mRNA-decapping enzyme subunit 2



#### 4.2.2 Score per residue for model 2

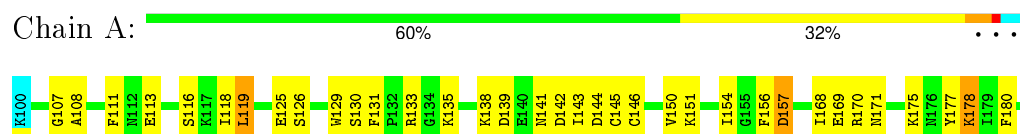
- Molecule 1: mRNA-decapping enzyme subunit 2





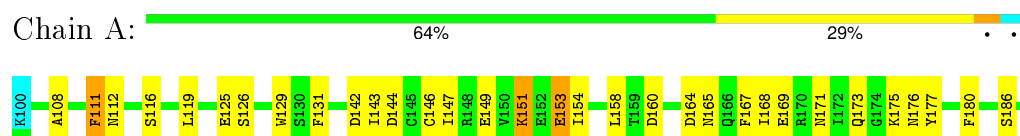
#### 4.2.3 Score per residue for model 3

- Molecule 1: mRNA-decapping enzyme subunit 2



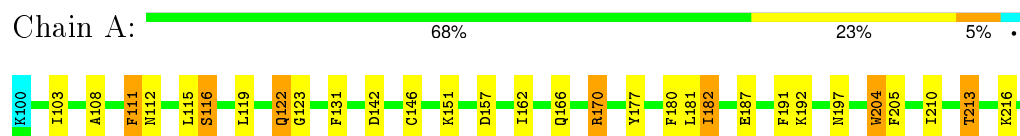
#### 4.2.4 Score per residue for model 4

- Molecule 1: mRNA-decapping enzyme subunit 2



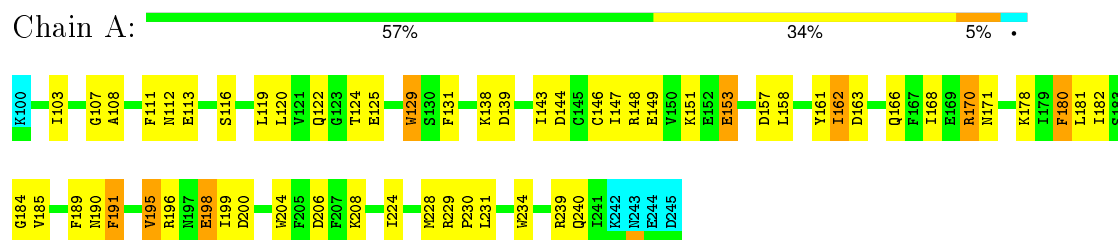
#### 4.2.5 Score per residue for model 5

- Molecule 1: mRNA-decapping enzyme subunit 2



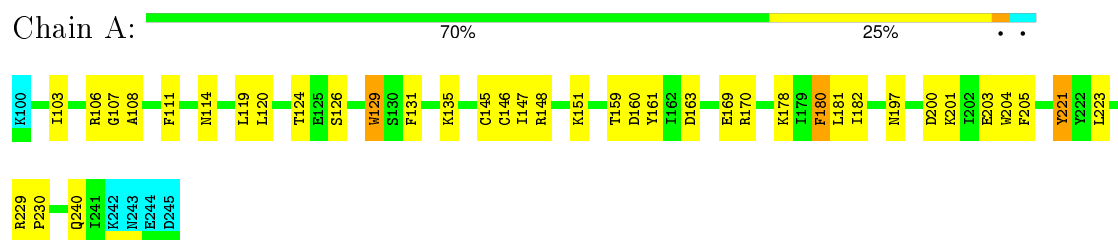
#### 4.2.6 Score per residue for model 6

- Molecule 1: mRNA-decapping enzyme subunit 2



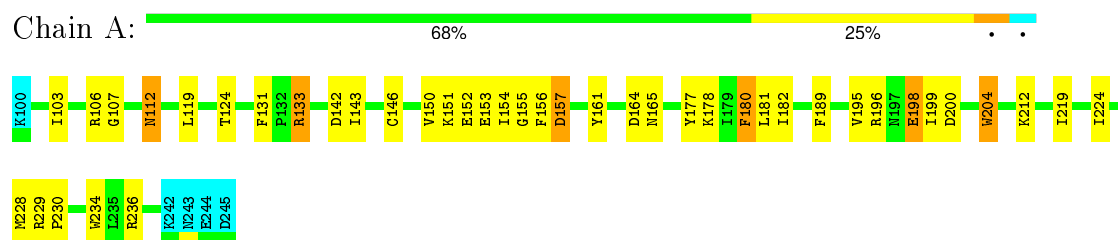
#### 4.2.7 Score per residue for model 7

- Molecule 1: mRNA-decapping enzyme subunit 2



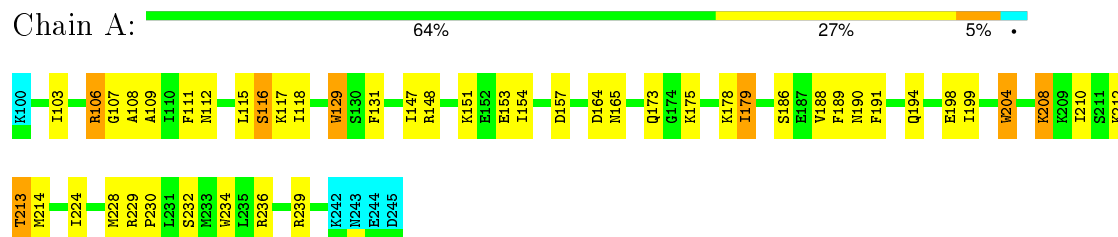
#### 4.2.8 Score per residue for model 8

- Molecule 1: mRNA-decapping enzyme subunit 2



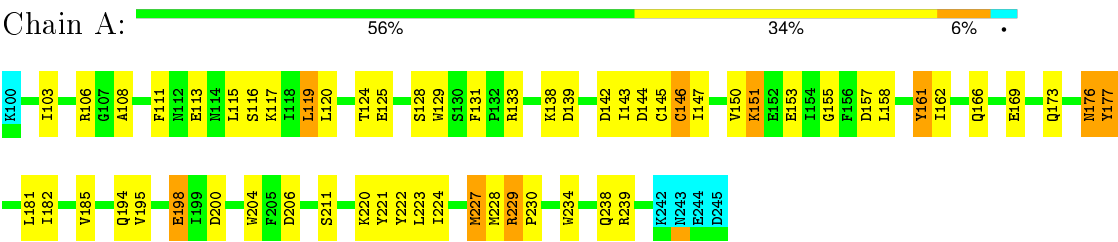
#### 4.2.9 Score per residue for model 9

- Molecule 1: mRNA-decapping enzyme subunit 2



4.2.10 Score per residue for model 10

- Molecule 1: mRNA-decapping enzyme subunit 2





## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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 ⓘ

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	1178	1181	1180	35±7
All	All	11780	11810	11800	347

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:HD22	1:A:120:LEU:N	0.77	1.95	1	2
1:A:110:ILE:HD13	1:A:110:ILE:N	0.73	1.97	1	1
1:A:158:LEU:N	1:A:158:LEU:HD12	0.73	1.98	10	2
1:A:106:ARG:HE	1:A:136:ILE:HD12	0.68	1.48	2	1
1:A:154:ILE:HG23	1:A:156:PHE:H	0.67	1.49	8	1
1:A:162:ILE:CG2	1:A:182:ILE:HG23	0.67	2.19	10	1
1:A:109:ALA:C	1:A:110:ILE:HD13	0.66	2.10	1	1
1:A:124:THR:HG22	1:A:198:GLU:OE1	0.66	1.91	10	1
1:A:103:ILE:O	1:A:103:ILE:HG23	0.64	1.91	6	4
1:A:111:PHE:N	1:A:111:PHE:CD1	0.63	2.67	1	2
1:A:109:ALA:HB3	1:A:180:PHE:O	0.63	1.94	2	1
1:A:195:VAL:HG23	1:A:196:ARG:N	0.63	2.07	6	1
1:A:166:GLN:NE2	1:A:234:TRP:NE1	0.62	2.47	6	1
1:A:146:CYS:O	1:A:150:VAL:HG23	0.62	1.95	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:VAL:HG12	1:A:196:ARG:N	0.62	2.10	3	1
1:A:112:ASN:HD22	1:A:112:ASN:N	0.62	1.93	1	1
1:A:117:LYS:NZ	1:A:204:TRP:CD1	0.61	2.68	9	1
1:A:111:PHE:CD1	1:A:111:PHE:N	0.61	2.66	5	2
1:A:218:ASN:OD1	1:A:219:ILE:HG22	0.60	1.96	1	1
1:A:112:ASN:HD21	1:A:116:SER:N	0.60	1.94	1	2
1:A:191:PHE:N	1:A:191:PHE:CD1	0.60	2.70	6	1
1:A:129:TRP:NE1	1:A:221:TYR:CE1	0.59	2.70	2	1
1:A:146:CYS:SG	1:A:180:PHE:CE1	0.59	2.96	7	2
1:A:227:MET:N	1:A:227:MET:SD	0.59	2.76	3	1
1:A:106:ARG:NH1	1:A:145:CYS:SG	0.59	2.76	10	1
1:A:192:LYS:CD	1:A:192:LYS:N	0.59	2.65	3	1
1:A:146:CYS:SG	1:A:180:PHE:CZ	0.59	2.95	7	2
1:A:133:ARG:N	1:A:133:ARG:CD	0.59	2.66	1	1
1:A:103:ILE:HG23	1:A:103:ILE:O	0.58	1.97	9	1
1:A:112:ASN:ND2	1:A:112:ASN:N	0.58	2.50	1	1
1:A:145:CYS:SG	1:A:146:CYS:N	0.58	2.76	10	1
1:A:146:CYS:SG	1:A:180:PHE:CD2	0.58	2.96	4	3
1:A:154:ILE:HD12	1:A:154:ILE:N	0.57	2.13	4	1
1:A:162:ILE:HD13	1:A:163:ASP:N	0.57	2.14	6	1
1:A:223:LEU:N	1:A:223:LEU:HD12	0.57	2.14	5	1
1:A:166:GLN:NE2	1:A:234:TRP:HE1	0.57	1.98	6	1
1:A:182:ILE:O	1:A:182:ILE:HG23	0.57	1.99	6	1
1:A:158:LEU:CD1	1:A:158:LEU:N	0.56	2.68	10	1
1:A:112:ASN:HD21	1:A:116:SER:H	0.56	1.44	1	5
1:A:146:CYS:SG	1:A:180:PHE:CG	0.56	2.98	6	3
1:A:162:ILE:HG22	1:A:182:ILE:HG23	0.56	1.77	10	1
1:A:158:LEU:N	1:A:158:LEU:CD1	0.56	2.69	4	1
1:A:231:LEU:HD23	1:A:231:LEU:C	0.56	2.20	1	1
1:A:176:ASN:ND2	1:A:176:ASN:N	0.56	2.54	10	1
1:A:146:CYS:HG	1:A:180:PHE:CB	0.55	2.13	6	1
1:A:146:CYS:SG	1:A:180:PHE:CE2	0.55	2.99	7	1
1:A:129:TRP:NE1	1:A:221:TYR:CD1	0.55	2.74	2	1
1:A:146:CYS:SG	1:A:180:PHE:CD1	0.55	3.00	7	1
1:A:224:ILE:O	1:A:228:MET:N	0.55	2.40	2	9
1:A:221:TYR:CD1	1:A:221:TYR:N	0.55	2.73	1	1
1:A:119:LEU:O	1:A:131:PHE:CE1	0.54	2.60	5	6
1:A:106:ARG:O	1:A:106:ARG:NE	0.54	2.41	9	1
1:A:120:LEU:N	1:A:120:LEU:CD2	0.54	2.66	1	1
1:A:106:ARG:NH1	1:A:145:CYS:CB	0.54	2.71	10	1
1:A:180:PHE:CD1	1:A:180:PHE:O	0.54	2.60	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:PHE:O	1:A:189:PHE:CD1	0.54	2.61	3	1
1:A:181:LEU:O	1:A:182:ILE:HD12	0.54	2.03	5	1
1:A:108:ALA:O	1:A:131:PHE:CG	0.54	2.61	6	4
1:A:110:ILE:CD1	1:A:110:ILE:N	0.54	2.64	1	1
1:A:122:GLN:NE2	1:A:199:ILE:CG2	0.53	2.71	6	1
1:A:119:LEU:O	1:A:131:PHE:CZ	0.53	2.60	6	4
1:A:112:ASN:ND2	1:A:116:SER:H	0.53	2.00	9	5
1:A:156:PHE:CE2	1:A:157:ASP:O	0.53	2.62	1	1
1:A:215:TYR:CD2	1:A:215:TYR:O	0.53	2.62	2	2
1:A:133:ARG:NE	1:A:177:TYR:OH	0.53	2.41	10	1
1:A:107:GLY:N	1:A:178:LYS:O	0.53	2.41	3	6
1:A:157:ASP:N	1:A:157:ASP:OD1	0.53	2.42	3	1
1:A:112:ASN:ND2	1:A:116:SER:OG	0.53	2.41	4	1
1:A:142:ASP:OD1	1:A:143:ILE:N	0.53	2.42	10	3
1:A:146:CYS:SG	1:A:147:ILE:N	0.53	2.82	10	1
1:A:154:ILE:N	1:A:154:ILE:CD1	0.53	2.72	4	1
1:A:120:LEU:CD2	1:A:120:LEU:N	0.52	2.68	7	1
1:A:170:ARG:NH2	1:A:226:SER:OG	0.52	2.43	5	1
1:A:108:ALA:O	1:A:131:PHE:CD1	0.52	2.62	5	3
1:A:215:TYR:O	1:A:215:TYR:CD2	0.52	2.62	4	1
1:A:106:ARG:NE	1:A:136:ILE:HD12	0.52	2.18	2	1
1:A:124:THR:OG1	1:A:196:ARG:NH2	0.52	2.42	8	2
1:A:157:ASP:OD1	1:A:157:ASP:N	0.52	2.42	8	1
1:A:168:ILE:HD12	1:A:234:TRP:CD1	0.52	2.40	4	1
1:A:189:PHE:CE1	1:A:190:ASN:O	0.52	2.62	6	2
1:A:160:ASP:OD1	1:A:161:TYR:CD2	0.52	2.62	7	3
1:A:143:ILE:HG23	1:A:144:ASP:N	0.52	2.19	10	5
1:A:133:ARG:HE	1:A:133:ARG:H	0.52	1.48	8	1
1:A:115:LEU:N	1:A:115:LEU:HD22	0.52	2.20	10	1
1:A:186:SER:OG	1:A:188:VAL:HG22	0.52	2.04	9	1
1:A:167:PHE:CD2	1:A:169:GLU:OE2	0.52	2.62	4	1
1:A:195:VAL:HG12	1:A:196:ARG:H	0.52	1.64	3	1
1:A:115:LEU:N	1:A:115:LEU:CD2	0.52	2.73	10	1
1:A:198:GLU:CG	1:A:199:ILE:N	0.51	2.72	8	4
1:A:167:PHE:CE2	1:A:169:GLU:OE2	0.51	2.62	4	1
1:A:160:ASP:OD1	1:A:161:TYR:CE2	0.51	2.63	2	1
1:A:108:ALA:O	1:A:131:PHE:CD2	0.51	2.63	10	2
1:A:161:TYR:CD1	1:A:184:GLY:O	0.51	2.63	6	1
1:A:189:PHE:O	1:A:189:PHE:CG	0.51	2.64	3	1
1:A:115:LEU:HD21	1:A:235:LEU:HD12	0.51	1.81	5	1
1:A:164:ASP:N	1:A:164:ASP:OD1	0.50	2.44	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:ASP:N	1:A:200:ASP:OD1	0.50	2.43	8	2
1:A:176:ASN:N	1:A:176:ASN:HD22	0.50	2.02	10	1
1:A:219:ILE:HG23	1:A:219:ILE:O	0.50	2.07	8	2
1:A:170:ARG:NH2	1:A:226:SER:O	0.50	2.44	1	1
1:A:173:GLN:NE2	1:A:222:TYR:CE2	0.50	2.79	10	1
1:A:164:ASP:OD1	1:A:165:ASN:N	0.50	2.43	1	3
1:A:107:GLY:O	1:A:180:PHE:CE2	0.50	2.65	3	1
1:A:176:ASN:ND2	1:A:176:ASN:H	0.50	2.04	10	1
1:A:161:TYR:CE1	1:A:184:GLY:O	0.49	2.65	6	1
1:A:133:ARG:NE	1:A:133:ARG:O	0.49	2.45	8	1
1:A:142:ASP:O	1:A:146:CYS:SG	0.49	2.70	3	5
1:A:111:PHE:CE1	1:A:235:LEU:HD11	0.49	2.42	5	1
1:A:150:VAL:O	1:A:154:ILE:HG22	0.49	2.08	8	1
1:A:151:LYS:O	1:A:155:GLY:N	0.49	2.46	10	2
1:A:106:ARG:HH11	1:A:145:CYS:CB	0.49	2.21	10	1
1:A:153:GLU:O	1:A:194:GLN:N	0.49	2.44	10	1
1:A:117:LYS:NZ	1:A:206:ASP:OD2	0.49	2.46	10	1
1:A:162:ILE:HD13	1:A:163:ASP:H	0.49	1.67	6	1
1:A:119:LEU:O	1:A:120:LEU:HD22	0.49	2.08	10	2
1:A:201:LYS:NZ	1:A:203:GLU:OE2	0.49	2.45	7	1
1:A:108:ALA:O	1:A:131:PHE:CB	0.49	2.61	2	2
1:A:166:GLN:O	1:A:180:PHE:CE1	0.48	2.67	1	1
1:A:212:LYS:O	1:A:214:MET:N	0.48	2.42	3	2
1:A:125:GLU:CD	1:A:125:GLU:H	0.48	2.11	6	2
1:A:164:ASP:OD1	1:A:164:ASP:N	0.48	2.47	8	1
1:A:176:ASN:ND2	1:A:176:ASN:O	0.48	2.47	10	1
1:A:154:ILE:HG23	1:A:156:PHE:N	0.48	2.23	8	1
1:A:103:ILE:O	1:A:103:ILE:CG2	0.48	2.62	6	3
1:A:231:LEU:O	1:A:231:LEU:HD23	0.48	2.08	1	1
1:A:154:ILE:CG2	1:A:156:PHE:O	0.48	2.62	8	1
1:A:108:ALA:HB2	1:A:180:PHE:CZ	0.47	2.44	5	1
1:A:195:VAL:CG1	1:A:196:ARG:N	0.47	2.77	3	1
1:A:213:THR:O	1:A:216:LYS:N	0.47	2.48	4	1
1:A:156:PHE:CD2	1:A:189:PHE:CE2	0.47	3.02	3	1
1:A:133:ARG:CZ	1:A:133:ARG:O	0.47	2.63	8	1
1:A:168:ILE:HD11	1:A:181:LEU:HD11	0.47	1.86	6	1
1:A:223:LEU:HD12	1:A:223:LEU:N	0.47	2.23	7	1
1:A:119:LEU:O	1:A:131:PHE:CE2	0.47	2.68	3	1
1:A:238:GLN:C	1:A:240:GLN:N	0.47	2.68	2	1
1:A:129:TRP:CE3	1:A:221:TYR:CZ	0.47	3.03	10	1
1:A:160:ASP:OD1	1:A:161:TYR:CZ	0.47	2.67	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:GLU:CG	1:A:169:GLU:O	0.47	2.62	10	1
1:A:169:GLU:N	1:A:169:GLU:CD	0.47	2.68	4	1
1:A:166:GLN:NE2	1:A:234:TRP:CE2	0.47	2.83	6	1
1:A:222:TYR:CG	1:A:223:LEU:N	0.47	2.83	10	1
1:A:147:ILE:O	1:A:151:LYS:CG	0.46	2.63	4	1
1:A:206:ASP:OD1	1:A:207:PHE:N	0.46	2.49	1	1
1:A:221:TYR:N	1:A:221:TYR:CD1	0.46	2.82	7	1
1:A:151:LYS:CG	1:A:152:GLU:N	0.46	2.79	8	1
1:A:229:ARG:CB	1:A:230:PRO:CD	0.46	2.94	4	9
1:A:115:LEU:O	1:A:239:ARG:NH1	0.46	2.49	9	1
1:A:225:ASN:CG	1:A:226:SER:N	0.46	2.69	4	1
1:A:146:CYS:SG	1:A:180:PHE:CB	0.46	3.04	6	1
1:A:166:GLN:HG2	1:A:181:LEU:HD12	0.46	1.87	10	1
1:A:154:ILE:HD13	1:A:191:PHE:CE2	0.46	2.45	9	1
1:A:195:VAL:CG2	1:A:196:ARG:N	0.46	2.74	6	1
1:A:112:ASN:ND2	1:A:204:TRP:CE2	0.46	2.83	8	1
1:A:180:PHE:N	1:A:180:PHE:CD1	0.46	2.82	8	2
1:A:187:GLU:OE1	1:A:204:TRP:CZ2	0.46	2.69	5	1
1:A:147:ILE:HG23	1:A:148:ARG:N	0.45	2.26	9	2
1:A:150:VAL:HG13	1:A:154:ILE:HD12	0.45	1.88	1	2
1:A:112:ASN:OD1	1:A:116:SER:N	0.45	2.49	2	4
1:A:238:GLN:O	1:A:240:GLN:N	0.45	2.49	2	1
1:A:147:ILE:CG2	1:A:148:ARG:N	0.45	2.80	9	3
1:A:143:ILE:CG2	1:A:144:ASP:N	0.45	2.79	6	3
1:A:212:LYS:C	1:A:214:MET:N	0.45	2.69	9	1
1:A:232:SER:O	1:A:236:ARG:CG	0.45	2.64	9	1
1:A:169:GLU:OE1	1:A:170:ARG:N	0.45	2.49	2	1
1:A:158:LEU:HD23	1:A:161:TYR:HB3	0.45	1.88	10	1
1:A:129:TRP:N	1:A:129:TRP:CD1	0.45	2.85	3	1
1:A:218:ASN:N	1:A:218:ASN:OD1	0.45	2.49	2	1
1:A:138:LYS:O	1:A:139:ASP:CB	0.45	2.64	10	3
1:A:166:GLN:HE22	1:A:238:GLN:CD	0.45	2.15	5	1
1:A:223:LEU:CD1	1:A:223:LEU:N	0.45	2.80	5	1
1:A:189:PHE:CD1	1:A:190:ASN:N	0.45	2.85	9	1
1:A:157:ASP:O	1:A:157:ASP:OD1	0.44	2.36	1	4
1:A:146:CYS:O	1:A:150:VAL:CG2	0.44	2.64	10	1
1:A:228:MET:SD	1:A:228:MET:C	0.44	2.96	9	1
1:A:181:LEU:HD12	1:A:234:TRP:CD1	0.44	2.48	8	1
1:A:208:LYS:N	1:A:208:LYS:CD	0.44	2.80	9	1
1:A:162:ILE:HG23	1:A:162:ILE:O	0.44	2.11	2	1
1:A:154:ILE:CG2	1:A:156:PHE:H	0.44	2.24	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:MET:SD	1:A:227:MET:N	0.44	2.90	10	1
1:A:210:ILE:O	1:A:213:THR:CG2	0.44	2.66	9	1
1:A:210:ILE:O	1:A:213:THR:OG1	0.44	2.36	5	1
1:A:122:GLN:OE1	1:A:123:GLY:O	0.44	2.36	5	1
1:A:166:GLN:HE22	1:A:238:GLN:CG	0.43	2.26	5	1
1:A:209:LYS:O	1:A:213:THR:N	0.43	2.42	2	1
1:A:133:ARG:CZ	1:A:177:TYR:OH	0.43	2.67	3	1
1:A:157:ASP:OD1	1:A:157:ASP:O	0.43	2.36	9	1
1:A:215:TYR:O	1:A:215:TYR:CG	0.43	2.71	4	1
1:A:160:ASP:OD1	1:A:160:ASP:O	0.43	2.37	4	1
1:A:113:GLU:OE2	1:A:185:VAL:O	0.43	2.37	6	1
1:A:149:GLU:O	1:A:153:GLU:OE2	0.43	2.36	4	1
1:A:133:ARG:NE	1:A:133:ARG:C	0.43	2.72	8	1
1:A:133:ARG:O	1:A:153:GLU:OE2	0.43	2.37	8	1
1:A:234:TRP:O	1:A:238:GLN:OE1	0.43	2.37	10	1
1:A:163:ASP:OD2	1:A:181:LEU:O	0.43	2.36	2	2
1:A:170:ARG:O	1:A:177:TYR:O	0.43	2.37	3	1
1:A:171:ASN:OD1	1:A:175:LYS:O	0.43	2.37	3	1
1:A:166:GLN:HE21	1:A:234:TRP:HE1	0.43	1.50	6	1
1:A:212:LYS:C	1:A:214:MET:H	0.43	2.17	9	1
1:A:113:GLU:CG	1:A:185:VAL:O	0.43	2.66	10	1
1:A:149:GLU:O	1:A:153:GLU:OE1	0.43	2.37	6	1
1:A:112:ASN:OD1	1:A:115:LEU:N	0.42	2.52	5	1
1:A:146:CYS:O	1:A:150:VAL:N	0.42	2.50	1	1
1:A:221:TYR:O	1:A:225:ASN:CB	0.42	2.67	5	1
1:A:200:ASP:O	1:A:200:ASP:OD1	0.42	2.37	6	2
1:A:176:ASN:O	1:A:176:ASN:OD1	0.42	2.37	4	1
1:A:109:ALA:HB2	1:A:179:ILE:CG1	0.42	2.44	9	1
1:A:153:GLU:O	1:A:194:GLN:OE1	0.42	2.36	9	1
1:A:212:LYS:O	1:A:213:THR:OG1	0.42	2.37	2	1
1:A:198:GLU:CG	1:A:199:ILE:H	0.42	2.27	3	3
1:A:229:ARG:HH11	1:A:229:ARG:CG	0.42	2.27	10	1
1:A:229:ARG:CG	1:A:229:ARG:NH1	0.42	2.80	10	1
1:A:129:TRP:CD1	1:A:129:TRP:N	0.42	2.85	7	1
1:A:129:TRP:CE3	1:A:205:PHE:CE2	0.42	3.08	7	1
1:A:122:GLN:HE22	1:A:199:ILE:CG2	0.42	2.27	6	1
1:A:229:ARG:N	1:A:230:PRO:CD	0.42	2.83	7	1
1:A:129:TRP:CD2	1:A:129:TRP:N	0.42	2.87	9	1
1:A:112:ASN:CG	1:A:116:SER:H	0.42	2.17	5	1
1:A:168:ILE:HG22	1:A:169:GLU:N	0.42	2.29	3	1
1:A:119:LEU:C	1:A:120:LEU:HD22	0.42	2.35	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:ASN:O	1:A:145:CYS:SG	0.42	2.78	3	1
1:A:128:SER:C	1:A:129:TRP:CG	0.41	2.94	1	1
1:A:198:GLU:OE2	1:A:199:ILE:O	0.41	2.38	6	1
1:A:173:GLN:C	1:A:175:LYS:H	0.41	2.17	2	3
1:A:216:LYS:O	1:A:216:LYS:CG	0.41	2.68	5	1
1:A:131:PHE:O	1:A:133:ARG:NH1	0.41	2.53	1	1
1:A:112:ASN:CG	1:A:117:LYS:H	0.41	2.19	9	1
1:A:106:ARG:O	1:A:133:ARG:CB	0.41	2.69	8	1
1:A:181:LEU:CD1	1:A:234:TRP:CD1	0.41	3.04	8	1
1:A:231:LEU:C	1:A:231:LEU:CD2	0.41	2.89	1	1
1:A:113:GLU:OE2	1:A:184:GLY:O	0.41	2.39	6	1
1:A:238:GLN:N	1:A:238:GLN:CD	0.41	2.74	10	1
1:A:125:GLU:OE1	1:A:128:SER:CB	0.41	2.69	10	1
1:A:106:ARG:NH1	1:A:107:GLY:O	0.40	2.53	7	1
1:A:112:ASN:ND2	1:A:115:LEU:CA	0.40	2.85	1	1
1:A:164:ASP:CG	1:A:165:ASN:H	0.40	2.20	9	1
1:A:120:LEU:HD12	1:A:129:TRP:C	0.40	2.36	6	1
1:A:157:ASP:C	1:A:158:LEU:HD12	0.40	2.37	10	1
1:A:215:TYR:CG	1:A:215:TYR:O	0.40	2.74	2	1
1:A:170:ARG:C	1:A:171:ASN:HD22	0.40	2.19	6	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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	141/146 (97%)	127±2 (90±2%)	12±2 (8±1%)	2±1 (1±1%)	19	64
All	All	1410/1460 (97%)	1271 (90%)	119 (8%)	20 (1%)	19	64

All 7 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	198	GLU	7
1	A	126	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	213	THR	2
1	A	197	ASN	2
1	A	125	GLU	2
1	A	195	VAL	2
1	A	239	ARG	1

### 6.3.2 Protein sidechains ⓘ

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	133/138 (96%)	119±3 (89±2%)	14±3 (11±2%)	12	56
All	All	1330/1380 (96%)	1186 (89%)	144 (11%)	12	56

All 65 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	204	TRP	10
1	A	111	PHE	8
1	A	151	LYS	8
1	A	129	TRP	5
1	A	116	SER	5
1	A	177	TYR	5
1	A	192	LYS	4
1	A	182	ILE	4
1	A	229	ARG	4
1	A	221	TYR	3
1	A	170	ARG	3
1	A	195	VAL	3
1	A	180	PHE	3
1	A	103	ILE	3
1	A	130	SER	3
1	A	236	ARG	3
1	A	146	CYS	2
1	A	157	ASP	2
1	A	213	THR	2
1	A	133	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	153	GLU	2
1	A	118	ILE	2
1	A	234	TRP	2
1	A	161	TYR	2
1	A	145	CYS	2
1	A	198	GLU	2
1	A	162	ILE	2
1	A	119	LEU	2
1	A	135	LYS	2
1	A	191	PHE	2
1	A	231	LEU	2
1	A	169	GLU	2
1	A	208	LYS	2
1	A	220	LYS	2
1	A	112	ASN	2
1	A	200	ASP	2
1	A	227	MET	2
1	A	212	LYS	1
1	A	114	ASN	1
1	A	102	SER	1
1	A	194	GLN	1
1	A	176	ASN	1
1	A	179	ILE	1
1	A	113	GLU	1
1	A	178	LYS	1
1	A	199	ILE	1
1	A	239	ARG	1
1	A	205	PHE	1
1	A	186	SER	1
1	A	218	ASN	1
1	A	124	THR	1
1	A	215	TYR	1
1	A	185	VAL	1
1	A	110	ILE	1
1	A	171	ASN	1
1	A	122	GLN	1
1	A	187	GLU	1
1	A	189	PHE	1
1	A	206	ASP	1
1	A	211	SER	1
1	A	106	ARG	1
1	A	197	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	159	THR	1
1	A	158	LEU	1
1	A	225	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 carbohydrates 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

No chemical shift data were provided