



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:58 am GMT

PDB ID : 2OSG  
Title : Solution Structure and Binding Property of the Domain-swapped Dimer of ZO2PDZ2  
Authors : Wu, J.W.; Yang, Y.S.; Zhang, J.H.; Ji, P.; Wu, J.H.; Shi, Y.Y.  
Deposited on : 2007-02-05

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  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

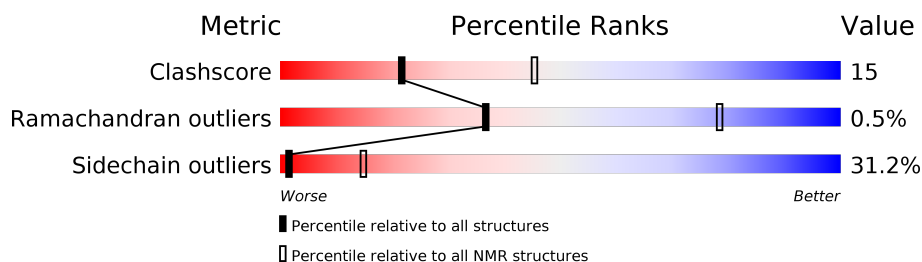
# 1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	83	 48% 36% • 13%
1	B	83	 45% 40% • 13%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:2-A:8, A:14-A:78, B:85-B:91, B:97-B:161 (144)	0.36	19

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2674 atoms, of which 1382 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tight junction protein ZO-2.

Mol	Chain	Residues	Atoms						Trace
1	A	83	Total	C	H	N	O	S	0
			1337	402	691	116	124	4	
1	B	83	Total	C	H	N	O	S	0
			1337	402	691	116	124	4	

There are 6 discrepancies between the modelled and reference sequences:

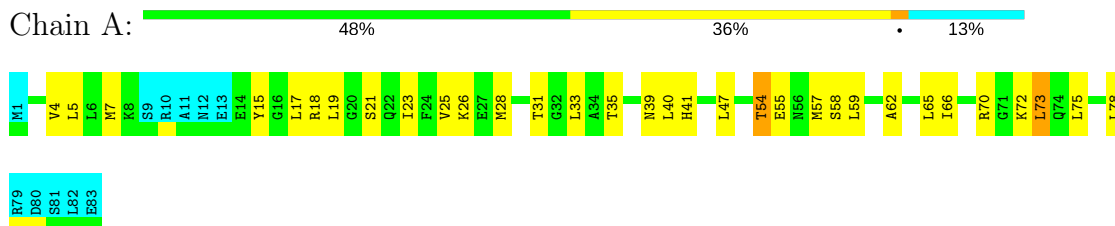
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q9UDY2
A	82	LEU	-	EXPRESSION TAG	UNP Q9UDY2
A	83	GLU	-	EXPRESSION TAG	UNP Q9UDY2
B	84	MET	-	INITIATING METHIONINE	UNP Q9UDY2
B	165	LEU	-	EXPRESSION TAG	UNP Q9UDY2
B	166	GLU	-	EXPRESSION TAG	UNP Q9UDY2

## 4 Residue-property plots

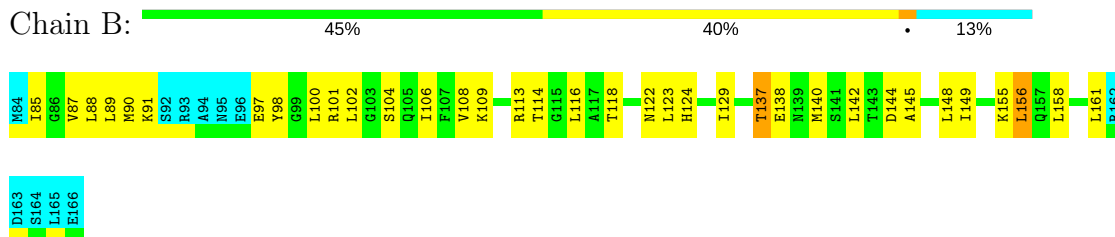
### 4.1 Average score per residue in the NMR ensemble

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: Tight junction protein ZO-2



- Molecule 1: Tight junction protein ZO-2

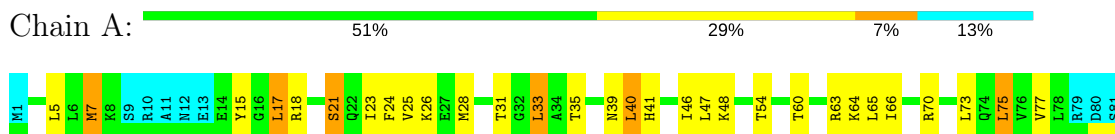


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

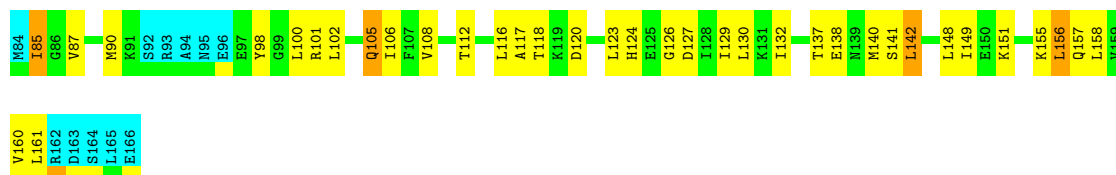
- Molecule 1: Tight junction protein ZO-2





- Molecule 1: Tight junction protein ZO-2

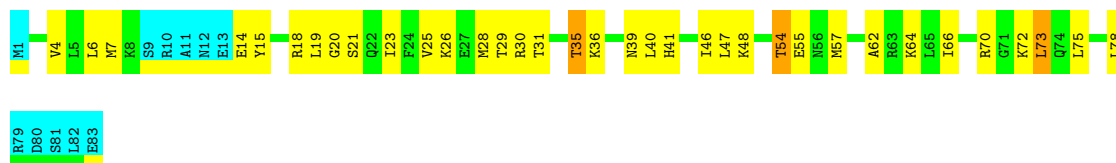
Chain B: 43% 39% 5% 13%



#### 4.2.2 Score per residue for model 2

- Molecule 1: Tight junction protein ZO-2

Chain A: 45% 39% 13%



- Molecule 1: Tight junction protein ZO-2

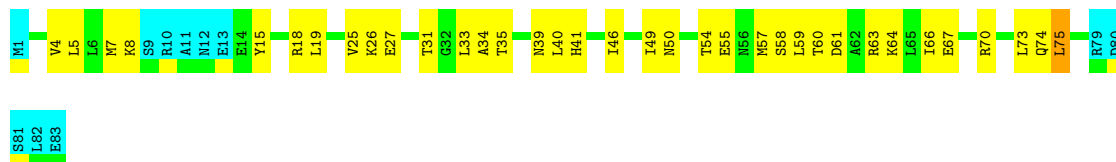
Chain B: 53% 29% 5% 13%



#### 4.2.3 Score per residue for model 3

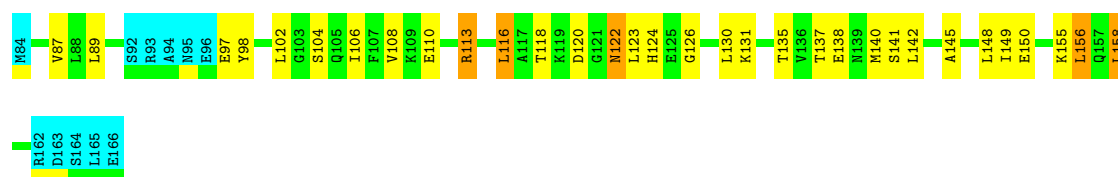
- Molecule 1: Tight junction protein ZO-2

Chain A: 45% 41% 13%



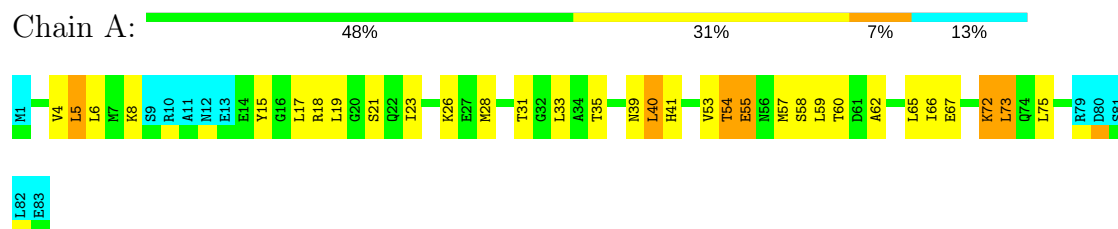
- Molecule 1: Tight junction protein ZO-2

Chain B: 48% 33% 6% 13%

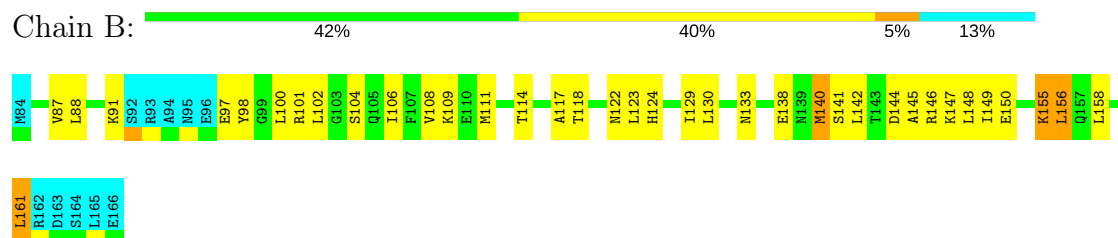


#### 4.2.4 Score per residue for model 4

- Molecule 1: Tight junction protein ZO-2

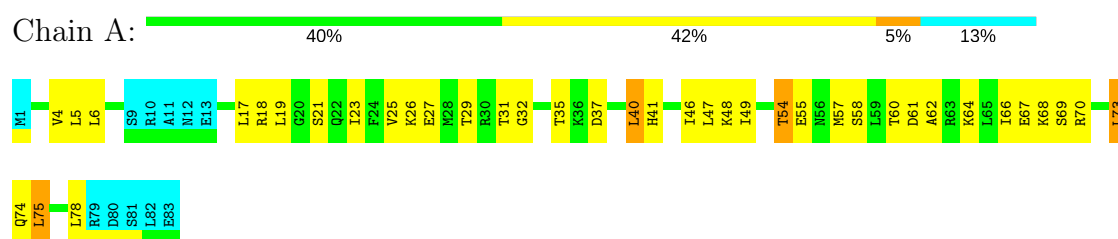


- Molecule 1: Tight junction protein ZO-2

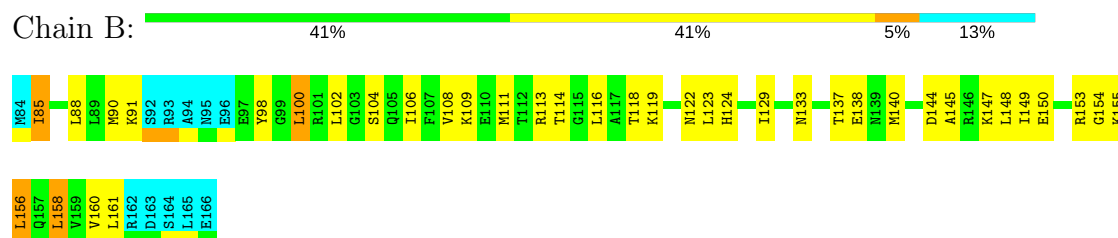


#### 4.2.5 Score per residue for model 5

- Molecule 1: Tight junction protein ZO-2

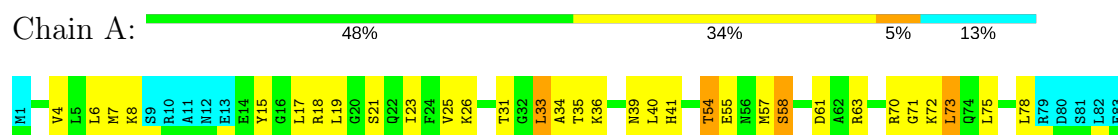


- Molecule 1: Tight junction protein ZO-2

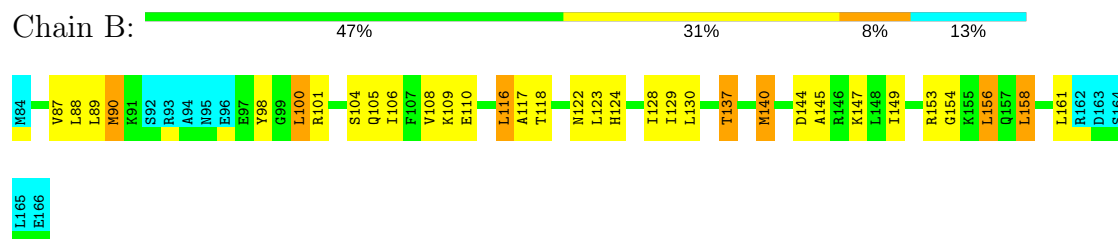


### 4.2.6 Score per residue for model 6

- Molecule 1: Tight junction protein ZO-2

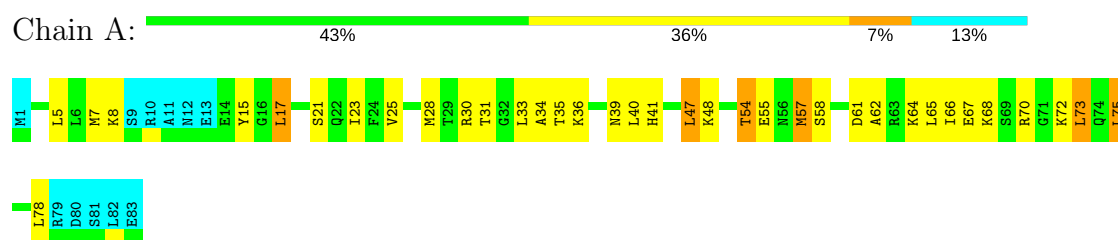


- Molecule 1: Tight junction protein ZO-2

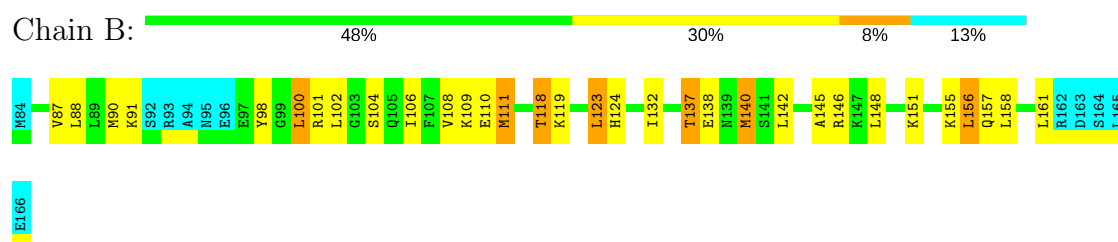


### 4.2.7 Score per residue for model 7

- Molecule 1: Tight junction protein ZO-2



- Molecule 1: Tight junction protein ZO-2

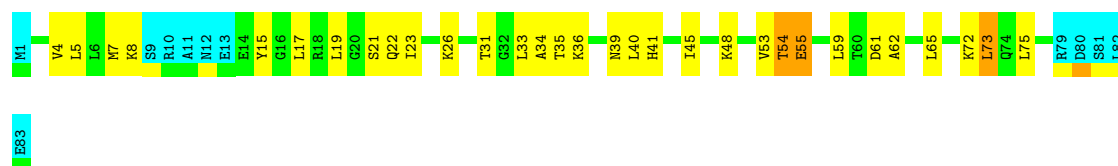


### 4.2.8 Score per residue for model 8

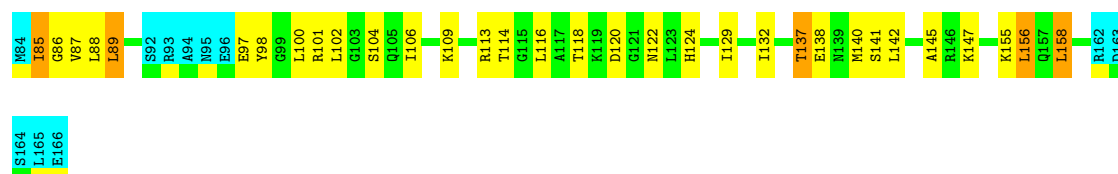
- Molecule 1: Tight junction protein ZO-2





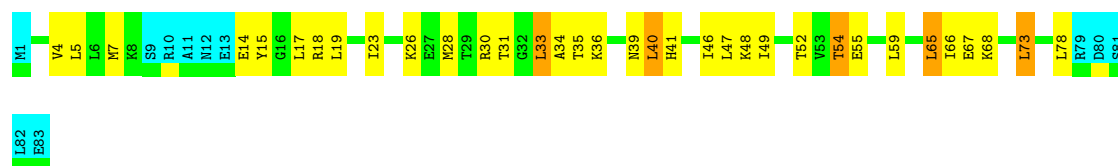


- Molecule 1: Tight junction protein ZO-2

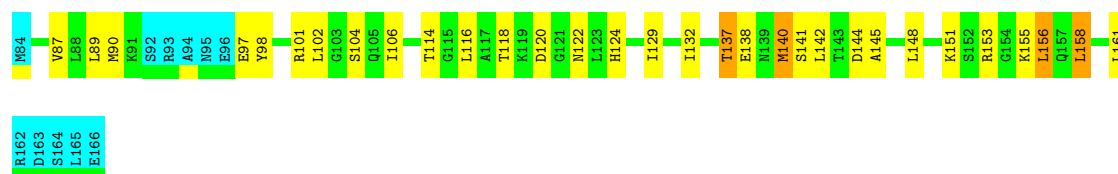


#### 4.2.9 Score per residue for model 9

- Molecule 1: Tight junction protein ZO-2

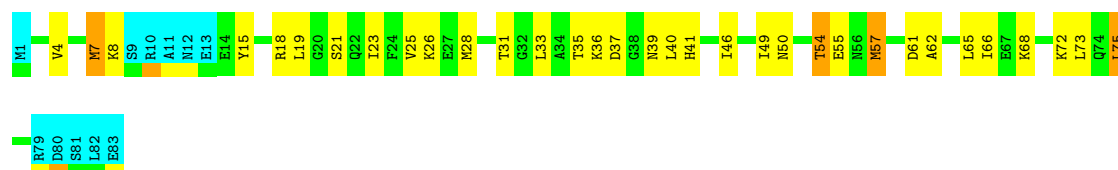


- Molecule 1: Tight junction protein ZO-2



#### 4.2.10 Score per residue for model 10

- Molecule 1: Tight junction protein ZO-2



- Molecule 1: Tight junction protein ZO-2

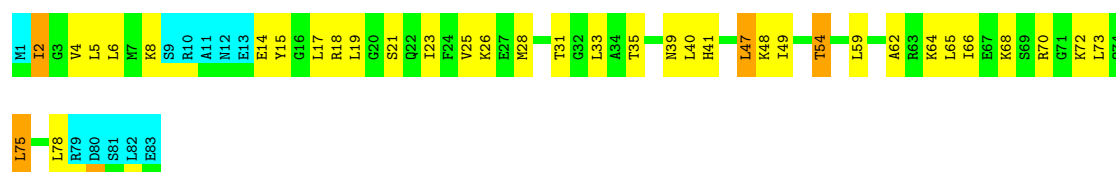
Chain B: 



#### 4.2.11 Score per residue for model 11

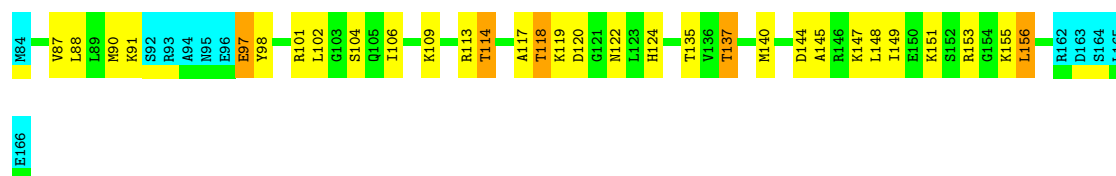
- Molecule 1: Tight junction protein ZO-2

Chain A: 



- Molecule 1: Tight junction protein ZO-2

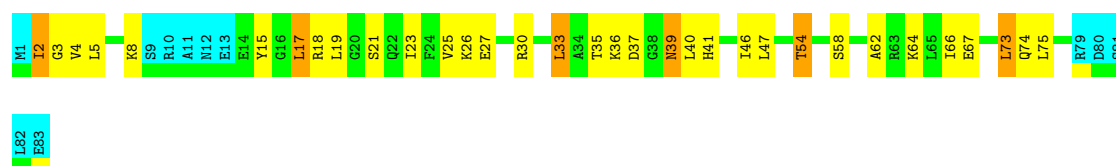
Chain B: 



#### 4.2.12 Score per residue for model 12

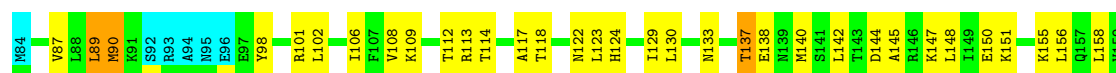
- Molecule 1: Tight junction protein ZO-2

Chain A: 



- Molecule 1: Tight junction protein ZO-2

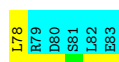
Chain B: 





#### 4.2.13 Score per residue for model 13

- Molecule 1: Tight junction protein ZO-2



- Molecule 1: Tight junction protein ZO-2

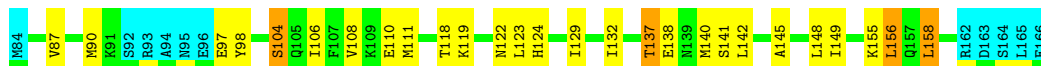


#### 4.2.14 Score per residue for model 14

- Molecule 1: Tight junction protein ZO-2

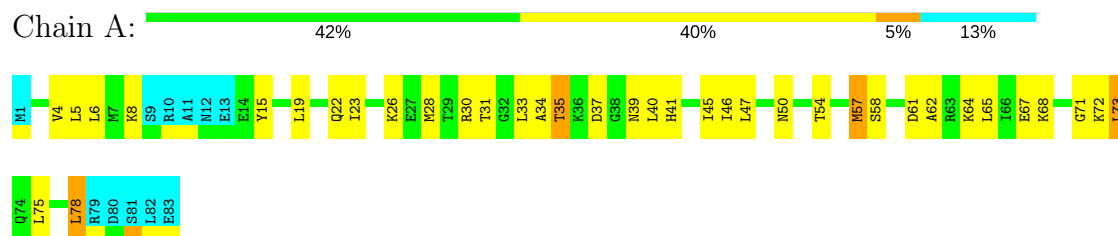


- Molecule 1: Tight junction protein ZO-2

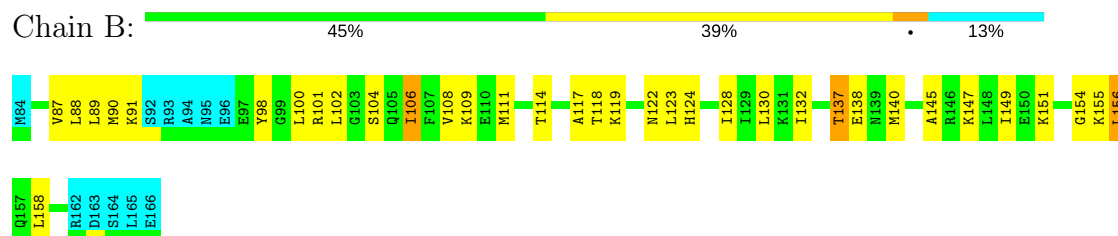


#### 4.2.15 Score per residue for model 15

- Molecule 1: Tight junction protein ZO-2

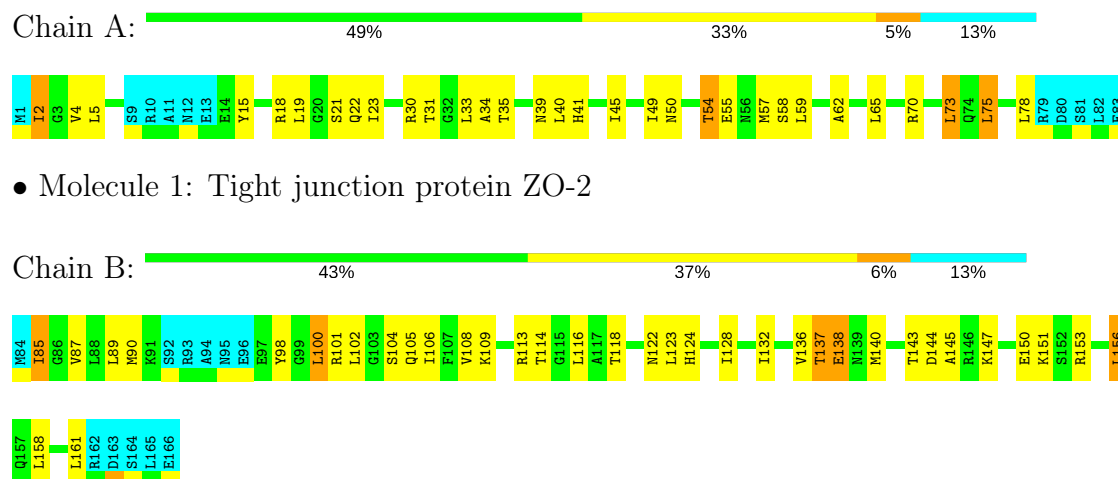


- Molecule 1: Tight junction protein ZO-2



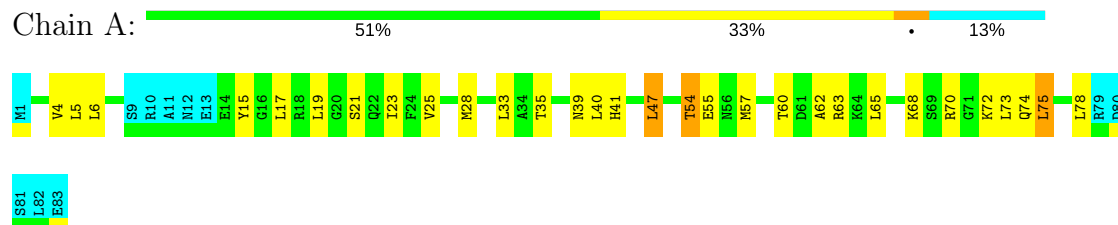
#### 4.2.16 Score per residue for model 16

- Molecule 1: Tight junction protein ZO-2

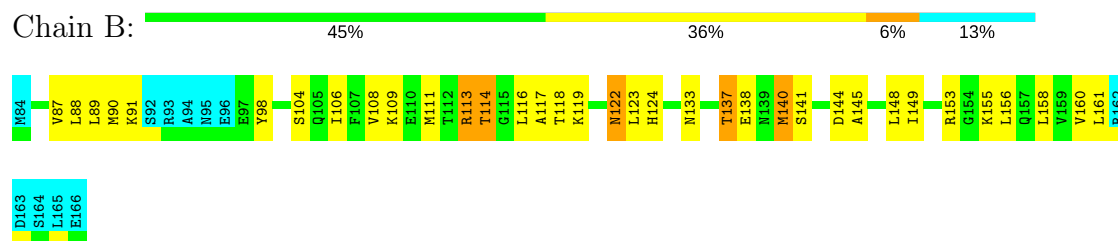


#### 4.2.17 Score per residue for model 17

- Molecule 1: Tight junction protein ZO-2

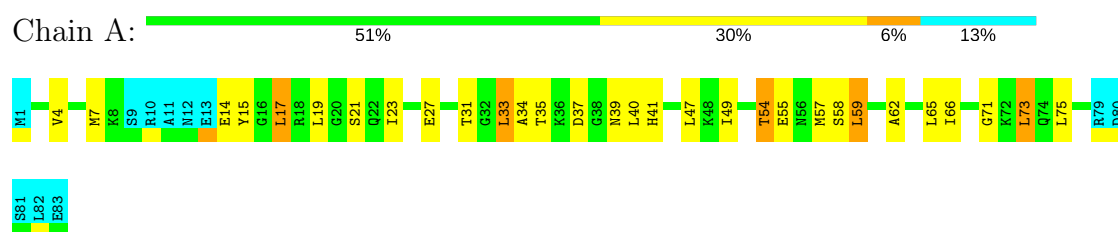


- Molecule 1: Tight junction protein ZO-2

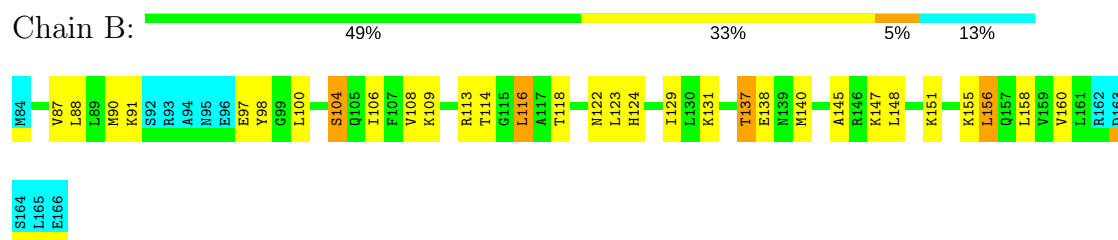


#### 4.2.18 Score per residue for model 18

- Molecule 1: Tight junction protein ZO-2

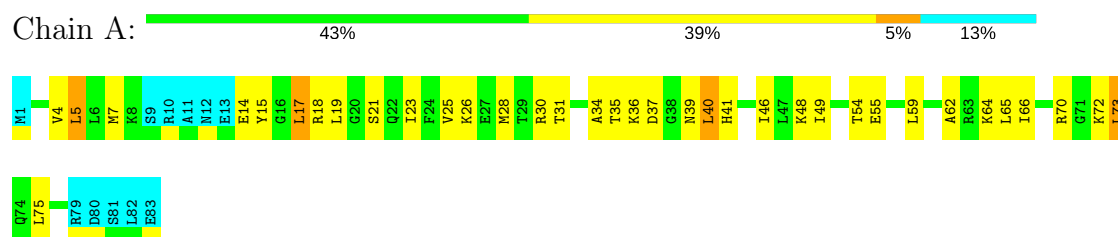


- Molecule 1: Tight junction protein ZO-2



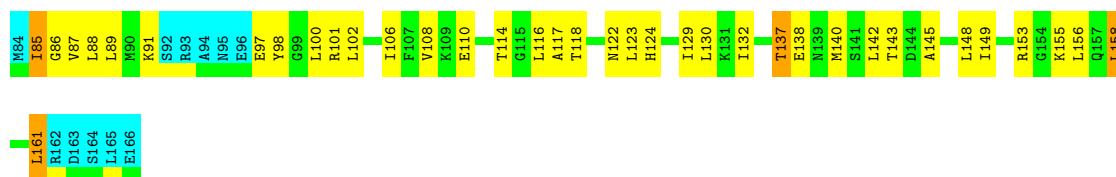
#### 4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: Tight junction protein ZO-2



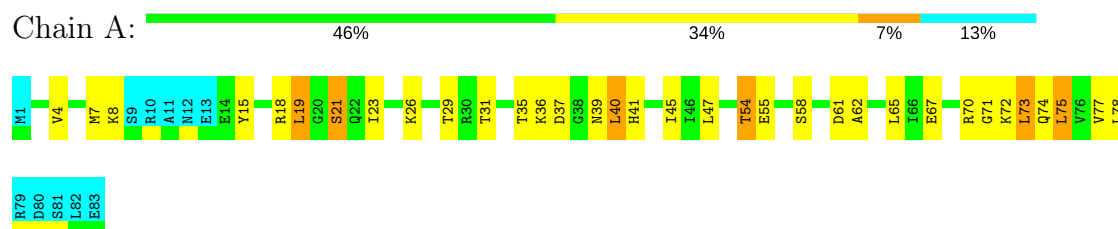
- Molecule 1: Tight junction protein ZO-2



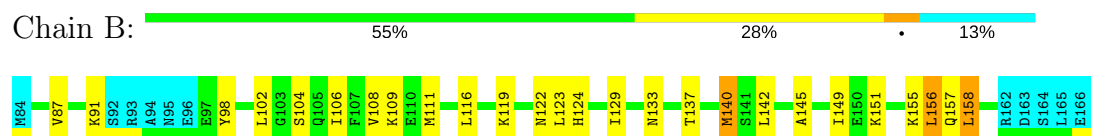


#### 4.2.20 Score per residue for model 20

- Molecule 1: Tight junction protein ZO-2



- Molecule 1: Tight junction protein ZO-2



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *distance geometry, simulated annealing, molecular dynamics*.

Of the 200 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	structure solution	1.1
CNS	refinement	1.1

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	556	606	605	23±4
1	B	556	606	605	25±5
All	All	22240	24240	24200	684

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:B:132:ILE:HD12	1:B:158:LEU:HD23	0.97	1.36	8	4
1:B:108:VAL:HG21	1:B:123:LEU:HD13	0.93	1.39	14	2
1:B:106:ILE:HD13	1:B:145:ALA:HB2	0.92	1.41	6	17
1:B:129:ILE:HG21	1:B:132:ILE:HD11	0.90	1.40	9	5
1:A:19:LEU:HD11	1:B:145:ALA:HB1	0.86	1.46	15	5
1:A:46:ILE:HG21	1:A:49:ILE:HD11	0.85	1.45	5	3
1:A:49:ILE:HD12	1:A:75:LEU:HD23	0.84	1.48	3	1
1:A:62:ALA:HB1	1:B:102:LEU:HD11	0.82	1.51	7	5
1:A:15:TYR:CE2	1:B:156:LEU:HD23	0.82	2.10	4	2
1:A:6:LEU:HD13	1:B:158:LEU:HD12	0.81	1.51	4	1
1:A:23:ILE:HD13	1:A:62:ALA:HB2	0.81	1.51	13	10
1:A:34:ALA:HB2	1:B:100:LEU:HD11	0.78	1.54	6	4
1:A:39:ASN:CB	1:B:87:VAL:HG11	0.77	2.08	8	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD13	1:A:78:LEU:HD21	0.77	1.55	2	1
1:A:15:TYR:CE1	1:B:156:LEU:HD23	0.77	2.15	17	4
1:A:73:LEU:HD23	1:B:98:TYR:CE2	0.76	2.15	1	4
1:A:40:LEU:HD11	1:A:75:LEU:HD22	0.76	1.58	15	4
1:A:73:LEU:HD23	1:B:98:TYR:CE1	0.75	2.16	10	4
1:A:25:VAL:HG21	1:A:40:LEU:HD13	0.74	1.59	5	1
1:B:106:ILE:HD12	1:B:137:THR:HG22	0.74	1.59	16	9
1:A:47:LEU:HD13	1:A:78:LEU:HD13	0.74	1.59	11	3
1:A:73:LEU:HD22	1:B:98:TYR:CZ	0.72	2.18	14	11
1:A:39:ASN:HB3	1:B:87:VAL:HG11	0.72	1.61	17	15
1:B:108:VAL:HG21	1:B:123:LEU:HB3	0.72	1.61	1	10
1:A:25:VAL:CG2	1:A:40:LEU:HD12	0.71	2.15	10	2
1:A:15:TYR:CZ	1:B:156:LEU:HD22	0.71	2.20	3	13
1:A:66:ILE:HD11	1:B:102:LEU:HD22	0.70	1.62	2	9
1:A:25:VAL:HG21	1:A:40:LEU:HD12	0.70	1.64	10	1
1:A:4:VAL:HG11	1:B:122:ASN:HB3	0.69	1.63	12	13
1:A:72:LYS:CG	1:B:88:LEU:HD21	0.69	2.17	4	1
1:A:19:LEU:HD22	1:B:149:ILE:HD11	0.69	1.62	3	10
1:B:108:VAL:HG21	1:B:123:LEU:CD1	0.69	2.18	14	1
1:A:23:ILE:HB	1:A:54:THR:HG22	0.68	1.66	14	16
1:B:106:ILE:HB	1:B:137:THR:HG22	0.68	1.63	10	10
1:A:47:LEU:HD13	1:A:78:LEU:HD11	0.68	1.65	9	1
1:A:47:LEU:HD13	1:A:78:LEU:HD22	0.68	1.65	5	1
1:A:25:VAL:HG21	1:A:40:LEU:HB3	0.67	1.66	3	9
1:A:40:LEU:HD11	1:A:75:LEU:HD13	0.67	1.66	3	3
1:B:123:LEU:HD11	1:B:158:LEU:HD22	0.67	1.67	18	2
1:B:129:ILE:HG21	1:B:132:ILE:CD1	0.67	2.18	9	1
1:B:123:LEU:HD11	1:B:158:LEU:HD13	0.67	1.67	6	2
1:A:4:VAL:HG11	1:B:122:ASN:CB	0.66	2.21	12	11
1:A:30:ARG:HA	1:A:35:THR:HG21	0.66	1.65	15	1
1:A:15:TYR:CD1	1:B:156:LEU:HD23	0.66	2.26	19	4
1:A:19:LEU:HD21	1:B:129:ILE:HD13	0.66	1.67	10	4
1:A:40:LEU:CD1	1:A:75:LEU:HD22	0.66	2.21	15	5
1:A:6:LEU:HD13	1:B:158:LEU:CD1	0.66	2.20	4	1
1:B:123:LEU:CD1	1:B:158:LEU:HD13	0.66	2.21	6	1
1:A:28:MET:SD	1:A:35:THR:HG23	0.65	2.30	2	2
1:B:129:ILE:HB	1:B:137:THR:HG21	0.64	1.67	1	4
1:A:23:ILE:CB	1:A:54:THR:HG22	0.64	2.21	9	4
1:B:106:ILE:CG1	1:B:137:THR:HG22	0.64	2.22	15	1
1:B:108:VAL:CG2	1:B:123:LEU:HD23	0.64	2.22	16	2
1:B:156:LEU:HD11	1:B:158:LEU:HD21	0.63	1.70	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:HD11	1:A:75:LEU:HD11	0.63	1.70	1	3
1:A:73:LEU:HD23	1:B:98:TYR:CD2	0.63	2.28	1	3
1:A:56:ASN:HA	1:B:142:LEU:HD21	0.63	1.71	13	1
1:A:39:ASN:HB3	1:B:87:VAL:HG21	0.63	1.69	8	2
1:A:7:MET:O	1:B:116:LEU:HD22	0.63	1.94	19	3
1:B:123:LEU:CD1	1:B:158:LEU:HD22	0.62	2.24	18	2
1:B:156:LEU:HD11	1:B:158:LEU:HD11	0.62	1.71	13	2
1:B:108:VAL:HG21	1:B:123:LEU:CD2	0.62	2.24	2	1
1:B:106:ILE:HG13	1:B:137:THR:HG22	0.62	1.70	15	1
1:B:106:ILE:CD1	1:B:137:THR:HG22	0.61	2.25	16	2
1:B:156:LEU:HD21	1:B:158:LEU:HD11	0.61	1.70	5	1
1:A:23:ILE:HD13	1:A:62:ALA:CB	0.61	2.25	19	6
1:B:106:ILE:HD13	1:B:145:ALA:CB	0.61	2.24	10	10
1:A:46:ILE:HG21	1:A:49:ILE:CD1	0.60	2.25	5	1
1:A:39:ASN:ND2	1:B:89:LEU:HD11	0.60	2.10	15	4
1:A:4:VAL:HG21	1:B:122:ASN:HB2	0.60	1.73	13	5
1:A:7:MET:O	1:B:116:LEU:HD13	0.60	1.96	6	6
1:A:40:LEU:HD21	1:A:77:VAL:HG22	0.59	1.73	1	1
1:B:132:ILE:CD1	1:B:158:LEU:HD23	0.59	2.26	14	4
1:A:15:TYR:CD2	1:B:156:LEU:HD23	0.59	2.32	4	2
1:A:17:LEU:HD21	1:B:123:LEU:HD11	0.59	1.74	7	1
1:A:73:LEU:HD23	1:B:98:TYR:CD1	0.59	2.33	6	4
1:A:17:LEU:HD22	1:B:123:LEU:HD22	0.58	1.74	17	1
1:A:5:LEU:HD22	1:B:155:LYS:HD2	0.58	1.75	4	1
1:A:59:LEU:HD11	1:B:102:LEU:O	0.58	1.99	19	1
1:B:113:ARG:HA	1:B:118:THR:HG21	0.58	1.74	13	5
1:A:2:ILE:HD13	1:A:3:GLY:N	0.58	2.14	14	2
1:A:6:LEU:HD23	1:A:15:TYR:CD2	0.58	2.34	17	2
1:A:75:LEU:HD13	1:B:89:LEU:HD13	0.58	1.75	6	1
1:A:39:ASN:CG	1:B:87:VAL:HG11	0.58	2.19	19	3
1:B:85:ILE:HD13	1:B:86:GLY:N	0.57	2.13	8	3
1:A:47:LEU:CD1	1:A:78:LEU:HD12	0.57	2.30	15	1
1:B:111:MET:SD	1:B:123:LEU:HD11	0.57	2.39	14	1
1:A:5:LEU:HD23	1:B:155:LYS:HD3	0.57	1.74	1	2
1:A:75:LEU:CD1	1:B:89:LEU:HD13	0.57	2.30	6	1
1:A:23:ILE:HD11	1:A:57:MET:HB3	0.57	1.76	10	2
1:A:6:LEU:HD11	1:B:122:ASN:ND2	0.57	2.14	4	2
1:A:39:ASN:OD1	1:B:87:VAL:HG11	0.57	1.99	9	2
1:A:17:LEU:HD21	1:B:117:ALA:CB	0.56	2.30	17	3
1:A:15:TYR:CE1	1:B:156:LEU:HD22	0.56	2.35	7	5
1:A:17:LEU:CD2	1:B:123:LEU:HD13	0.56	2.30	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:HD12	1:B:104:SER:OG	0.56	2.01	18	3
1:B:108:VAL:HG21	1:B:123:LEU:HD23	0.56	1.76	2	1
1:B:106:ILE:HD11	1:B:140:MET:HB3	0.56	1.77	5	9
1:A:40:LEU:CD1	1:A:75:LEU:HD13	0.56	2.30	18	2
1:A:73:LEU:HD11	1:A:75:LEU:HD21	0.56	1.76	11	2
1:A:46:ILE:HB	1:A:54:THR:HG21	0.55	1.76	13	2
1:A:33:LEU:HD22	1:B:90:MET:O	0.55	2.01	9	5
1:A:19:LEU:HD21	1:B:129:ILE:CD1	0.55	2.31	6	3
1:B:128:ILE:HD11	1:B:161:LEU:HB2	0.55	1.79	16	1
1:A:40:LEU:HD12	1:A:75:LEU:HD13	0.55	1.79	7	1
1:B:156:LEU:HD12	1:B:156:LEU:C	0.54	2.21	13	4
1:A:47:LEU:HD22	1:A:78:LEU:HD13	0.54	1.79	5	1
1:A:19:LEU:CD1	1:B:145:ALA:HB1	0.54	2.31	16	2
1:A:4:VAL:HG21	1:B:122:ASN:CB	0.54	2.33	17	5
1:A:39:ASN:CB	1:B:87:VAL:HG21	0.54	2.32	12	2
1:A:25:VAL:HG21	1:A:40:LEU:HG	0.54	1.80	13	1
1:A:75:LEU:N	1:A:75:LEU:HD22	0.54	2.17	13	1
1:A:49:ILE:HD13	1:A:75:LEU:HA	0.54	1.78	5	2
1:B:133:ASN:HB2	1:B:148:LEU:HD21	0.54	1.80	17	2
1:A:33:LEU:HD13	1:B:90:MET:O	0.53	2.03	18	5
1:A:25:VAL:HG13	1:B:100:LEU:CD2	0.53	2.34	5	1
1:B:158:LEU:N	1:B:158:LEU:HD22	0.53	2.17	20	1
1:B:106:ILE:HD12	1:B:137:THR:CG2	0.53	2.34	3	1
1:B:157:GLN:C	1:B:158:LEU:HD22	0.53	2.24	1	1
1:B:157:GLN:O	1:B:158:LEU:HD13	0.53	2.03	20	1
1:A:46:ILE:CG2	1:A:49:ILE:HD11	0.53	2.28	5	2
1:A:62:ALA:HB1	1:B:102:LEU:CD1	0.53	2.29	7	1
1:A:39:ASN:C	1:A:40:LEU:HD13	0.53	2.24	9	1
1:A:46:ILE:HD13	1:B:102:LEU:HD21	0.53	1.80	12	5
1:A:5:LEU:HD22	1:B:155:LYS:HE3	0.53	1.81	19	1
1:B:108:VAL:HG22	1:B:123:LEU:HD23	0.52	1.81	17	1
1:A:5:LEU:HD23	1:B:155:LYS:CD	0.52	2.35	13	1
1:B:130:LEU:HD13	1:B:161:LEU:HD13	0.52	1.81	19	2
1:B:156:LEU:HD21	1:B:158:LEU:CD1	0.52	2.34	5	1
1:A:23:ILE:HD12	1:A:54:THR:HG23	0.52	1.82	15	1
1:A:34:ALA:CB	1:B:100:LEU:HD11	0.51	2.34	13	2
1:A:73:LEU:C	1:A:73:LEU:HD12	0.51	2.25	3	3
1:B:89:LEU:HD23	1:B:98:TYR:CD1	0.51	2.41	12	1
1:B:106:ILE:HG21	1:B:145:ALA:HB1	0.51	1.82	2	1
1:A:46:ILE:HD11	1:B:102:LEU:HD11	0.51	1.83	10	1
1:B:123:LEU:CD2	1:B:158:LEU:HD13	0.51	2.35	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:123:LEU:HD11	1:B:129:ILE:HG12	0.51	1.82	1	1
1:A:22:GLN:NE2	1:A:45:ILE:HG21	0.51	2.21	16	3
1:B:106:ILE:HD11	1:B:140:MET:HG2	0.51	1.83	4	1
1:A:34:ALA:HA	1:B:89:LEU:HD21	0.51	1.83	19	1
1:A:62:ALA:O	1:A:66:ILE:HD12	0.51	2.06	18	1
1:B:114:THR:O	1:B:114:THR:HG23	0.50	2.06	17	1
1:A:73:LEU:O	1:A:73:LEU:HD23	0.50	2.07	12	3
1:B:129:ILE:HD13	1:B:160:VAL:HG12	0.50	1.83	18	1
1:A:34:ALA:CB	1:B:100:LEU:HD21	0.50	2.36	15	1
1:B:127:ASP:OD1	1:B:160:VAL:HG13	0.50	2.06	1	1
1:A:53:VAL:HG22	1:A:55:GLU:H	0.50	1.65	8	1
1:B:156:LEU:O	1:B:156:LEU:HD23	0.50	2.07	15	6
1:A:66:ILE:HG22	1:B:97:GLU:OE2	0.49	2.07	11	1
1:A:19:LEU:HD22	1:B:149:ILE:HD12	0.49	1.83	15	2
1:A:72:LYS:HD3	1:B:88:LEU:HD11	0.49	1.84	4	1
1:B:117:ALA:CB	1:B:123:LEU:HD12	0.49	2.37	12	1
1:A:34:ALA:N	1:B:89:LEU:HD21	0.49	2.22	8	3
1:B:130:LEU:HD13	1:B:161:LEU:HD12	0.49	1.84	12	1
1:A:47:LEU:HD13	1:A:78:LEU:HD12	0.49	1.84	15	1
1:B:106:ILE:HD12	1:B:137:THR:HG23	0.49	1.83	1	3
1:A:39:ASN:HB2	1:B:87:VAL:HG21	0.49	1.83	15	5
1:B:106:ILE:CD1	1:B:145:ALA:HB2	0.49	2.35	11	3
1:B:106:ILE:HG21	1:B:145:ALA:CB	0.49	2.37	2	1
1:A:49:ILE:CD1	1:A:75:LEU:HD23	0.49	2.30	3	1
1:A:73:LEU:HG	1:A:75:LEU:HD21	0.49	1.85	17	1
1:A:75:LEU:HD22	1:A:75:LEU:N	0.49	2.23	17	1
1:A:25:VAL:HG21	1:A:40:LEU:CD2	0.49	2.38	13	1
1:B:132:ILE:HG23	1:B:158:LEU:HD23	0.48	1.84	15	2
1:B:98:TYR:HB3	1:B:100:LEU:HD13	0.48	1.83	1	2
1:A:73:LEU:HD23	1:A:73:LEU:O	0.48	2.09	7	5
1:A:21:SER:OG	1:B:142:LEU:HD12	0.48	2.08	20	2
1:B:106:ILE:HB	1:B:137:THR:HG23	0.48	1.85	1	2
1:B:114:THR:HG23	1:B:114:THR:O	0.48	2.09	11	1
1:A:49:ILE:HD13	1:A:66:ILE:HD11	0.48	1.85	18	1
1:B:137:THR:HG22	1:B:137:THR:O	0.48	2.09	1	1
1:A:40:LEU:HD11	1:A:75:LEU:CB	0.48	2.38	20	1
1:A:46:ILE:CD1	1:B:102:LEU:HD21	0.47	2.39	1	2
1:A:74:GLN:O	1:A:75:LEU:HD13	0.47	2.09	13	2
1:A:25:VAL:HG21	1:A:40:LEU:CG	0.47	2.40	13	1
1:A:17:LEU:HD23	1:B:108:VAL:HG13	0.47	1.84	18	2
1:B:85:ILE:C	1:B:85:ILE:HD13	0.47	2.29	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LYS:HG3	1:B:88:LEU:HD21	0.47	1.86	4	1
1:A:47:LEU:HD13	1:A:78:LEU:CD1	0.47	2.40	17	2
1:A:21:SER:OG	1:B:142:LEU:HD11	0.47	2.09	14	1
1:A:46:ILE:HD12	1:B:102:LEU:HD21	0.47	1.86	13	1
1:A:19:LEU:HD12	1:B:106:ILE:HG21	0.47	1.87	18	1
1:A:47:LEU:HD12	1:A:78:LEU:HD13	0.47	1.87	7	1
1:B:113:ARG:O	1:B:114:THR:HG22	0.47	2.09	11	2
1:A:52:THR:HG21	1:A:65:LEU:HD11	0.47	1.87	9	1
1:A:2:ILE:HD13	1:A:2:ILE:C	0.47	2.30	14	2
1:B:123:LEU:HD11	1:B:158:LEU:CB	0.47	2.40	3	1
1:B:111:MET:SD	1:B:118:THR:HG23	0.46	2.50	7	1
1:A:40:LEU:HD12	1:A:75:LEU:HD22	0.46	1.87	11	2
1:A:23:ILE:HB	1:A:54:THR:HG23	0.46	1.85	15	1
1:A:40:LEU:HD11	1:A:75:LEU:HB2	0.46	1.86	20	1
1:A:40:LEU:CD2	1:A:75:LEU:HD13	0.46	2.40	10	1
1:A:50:ASN:HB2	1:A:65:LEU:HD11	0.46	1.87	15	1
1:B:132:ILE:HG22	1:B:133:ASN:HD22	0.46	1.70	13	1
1:A:17:LEU:HD11	1:B:117:ALA:HB2	0.46	1.86	11	1
1:A:23:ILE:HD11	1:A:57:MET:SD	0.46	2.50	15	1
1:A:25:VAL:CG2	1:A:40:LEU:HD22	0.46	2.40	19	1
1:A:17:LEU:HD11	1:B:117:ALA:CB	0.46	2.41	19	3
1:A:17:LEU:HD23	1:B:111:MET:CB	0.46	2.40	17	1
1:B:156:LEU:HD23	1:B:156:LEU:O	0.46	2.11	16	2
1:A:5:LEU:HD22	1:B:155:LYS:HG2	0.46	1.87	19	1
1:A:73:LEU:HD22	1:B:98:TYR:CE1	0.46	2.45	5	1
1:A:73:LEU:HD22	1:B:98:TYR:CE2	0.46	2.46	13	5
1:A:29:THR:HG23	1:A:32:GLY:HA3	0.45	1.87	5	1
1:B:85:ILE:HD13	1:B:85:ILE:C	0.45	2.32	5	2
1:A:73:LEU:HD12	1:A:73:LEU:C	0.45	2.32	1	1
1:A:17:LEU:HD21	1:B:117:ALA:HB2	0.45	1.88	17	2
1:A:5:LEU:HD23	1:B:155:LYS:NZ	0.45	2.25	17	1
1:A:65:LEU:HD23	1:A:65:LEU:C	0.45	2.32	13	1
1:B:123:LEU:HD21	1:B:158:LEU:HD13	0.45	1.89	12	1
1:B:158:LEU:CD2	1:B:160:VAL:HG13	0.45	2.42	12	2
1:A:73:LEU:CD1	1:A:75:LEU:HD11	0.45	2.41	1	1
1:B:156:LEU:HD21	1:B:158:LEU:CG	0.44	2.41	5	1
1:B:90:MET:HG3	1:B:91:LYS:N	0.44	2.27	7	2
1:A:65:LEU:C	1:A:65:LEU:HD23	0.44	2.32	4	2
1:A:17:LEU:HD22	1:B:123:LEU:HD13	0.44	1.88	12	1
1:A:66:ILE:CD1	1:B:102:LEU:HD22	0.44	2.43	9	2
1:A:4:VAL:HG11	1:B:122:ASN:HB2	0.44	1.89	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:123:LEU:HD12	1:B:123:LEU:C	0.44	2.33	14	1
1:A:74:GLN:C	1:A:75:LEU:HD13	0.44	2.33	17	1
1:A:15:TYR:CE2	1:B:156:LEU:HD22	0.44	2.47	15	1
1:B:148:LEU:HD23	1:B:148:LEU:C	0.44	2.32	4	1
1:A:39:ASN:CG	1:B:89:LEU:HD11	0.44	2.32	6	1
1:A:23:ILE:HB	1:A:54:THR:CG2	0.44	2.43	13	3
1:B:130:LEU:HD22	1:B:161:LEU:CD1	0.44	2.43	4	1
1:B:88:LEU:C	1:B:88:LEU:HD23	0.44	2.33	19	1
1:B:106:ILE:HB	1:B:137:THR:CG2	0.43	2.43	1	3
1:B:132:ILE:HG23	1:B:158:LEU:CD1	0.43	2.42	1	1
1:A:47:LEU:CD1	1:A:78:LEU:HD13	0.43	2.43	7	1
1:A:40:LEU:HD22	1:A:77:VAL:HG13	0.43	1.91	20	1
1:A:33:LEU:HD22	1:B:90:MET:H	0.43	1.73	15	1
1:A:40:LEU:HD22	1:A:77:VAL:CG1	0.43	2.43	20	1
1:A:65:LEU:O	1:A:65:LEU:HD23	0.43	2.13	10	1
1:B:156:LEU:HD11	1:B:158:LEU:CD1	0.43	2.42	13	1
1:A:57:MET:HG3	1:A:58:SER:N	0.43	2.27	6	1
1:A:33:LEU:O	1:B:89:LEU:HD11	0.43	2.12	13	1
1:A:49:ILE:HG22	1:A:50:ASN:HD22	0.43	1.72	16	1
1:A:19:LEU:HD22	1:B:149:ILE:CD1	0.43	2.44	5	1
1:B:156:LEU:CD1	1:B:158:LEU:HD21	0.43	2.43	10	1
1:B:148:LEU:C	1:B:148:LEU:HD23	0.43	2.33	5	2
1:A:73:LEU:HD23	1:B:98:TYR:CZ	0.43	2.49	6	1
1:B:108:VAL:O	1:B:126:GLY:N	0.43	2.51	1	2
1:B:142:LEU:HD23	1:B:142:LEU:O	0.43	2.13	4	1
1:A:7:MET:HG3	1:A:8:LYS:N	0.43	2.29	10	1
1:A:19:LEU:CD2	1:B:129:ILE:HD13	0.43	2.43	19	1
1:B:123:LEU:HD13	1:B:158:LEU:HD13	0.43	1.91	19	1
1:A:23:ILE:HD13	1:A:62:ALA:HB1	0.42	1.89	15	1
1:A:2:ILE:C	1:A:2:ILE:HD13	0.42	2.33	11	1
1:B:132:ILE:HG22	1:B:133:ASN:ND2	0.42	2.28	13	1
1:A:49:ILE:CD1	1:A:54:THR:HG21	0.42	2.45	11	1
1:A:75:LEU:HD12	1:B:87:VAL:O	0.42	2.15	8	1
1:B:113:ARG:CA	1:B:118:THR:HG21	0.42	2.43	13	1
1:A:49:ILE:HA	1:A:74:GLN:O	0.42	2.15	5	1
1:B:149:ILE:HG23	1:B:156:LEU:HD13	0.42	1.90	1	1
1:A:19:LEU:HD21	1:B:132:ILE:HD11	0.42	1.92	10	1
1:B:132:ILE:HA	1:B:157:GLN:O	0.42	2.15	7	1
1:A:4:VAL:HG21	1:B:122:ASN:HA	0.42	1.90	2	1
1:B:108:VAL:HG23	1:B:123:LEU:HD22	0.42	1.89	1	1
1:A:49:ILE:HD11	1:B:102:LEU:HD21	0.42	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:148:LEU:O	1:B:148:LEU:HD23	0.42	2.15	3	2
1:A:65:LEU:HD13	1:A:65:LEU:O	0.42	2.15	8	2
1:A:47:LEU:HD22	1:A:78:LEU:CD1	0.41	2.45	13	1
1:A:46:ILE:CD1	1:B:102:LEU:HD11	0.41	2.45	10	1
1:A:6:LEU:HD21	1:B:117:ALA:N	0.41	2.29	2	2
1:A:53:VAL:HG12	1:A:55:GLU:H	0.41	1.74	4	1
1:A:72:LYS:CD	1:B:88:LEU:HD21	0.41	2.45	4	1
1:B:123:LEU:HD11	1:B:158:LEU:HB2	0.41	1.91	19	1
1:A:34:ALA:HB3	1:B:100:LEU:HD11	0.41	1.91	18	1
1:A:15:TYR:HB3	1:A:17:LEU:HD13	0.41	1.90	11	1
1:A:54:THR:HG22	1:A:54:THR:O	0.41	2.15	15	1
1:A:20:GLY:O	1:B:106:ILE:HA	0.41	2.15	2	1
1:A:46:ILE:HD13	1:B:102:LEU:CD2	0.41	2.45	2	2
1:B:117:ALA:HB2	1:B:123:LEU:HD12	0.41	1.91	12	1
1:B:105:GLN:NE2	1:B:128:ILE:HG21	0.41	2.31	6	1
1:A:6:LEU:HD21	1:B:117:ALA:HB2	0.41	1.93	13	1
1:B:133:ASN:HB3	1:B:148:LEU:HD11	0.41	1.91	2	1
1:B:122:ASN:ND2	1:B:158:LEU:HD13	0.41	2.31	10	1
1:B:136:VAL:HG12	1:B:138:GLU:H	0.41	1.75	16	1
1:B:132:ILE:HD13	1:B:158:LEU:HA	0.41	1.92	19	1
1:A:24:PHE:CE1	1:B:105:GLN:CG	0.41	3.04	1	1
1:A:66:ILE:HD12	1:B:102:LEU:HD22	0.41	1.92	7	1
1:A:40:LEU:HD11	1:A:75:LEU:CD1	0.41	2.42	3	1
1:A:23:ILE:CD1	1:A:62:ALA:HB2	0.41	2.42	12	1
1:A:19:LEU:HD12	1:B:106:ILE:CG2	0.40	2.46	18	1
1:B:122:ASN:CG	1:B:123:LEU:HD13	0.40	2.37	2	1
1:A:49:ILE:HG22	1:A:50:ASN:ND2	0.40	2.31	16	1
1:B:149:ILE:HG23	1:B:156:LEU:HD22	0.40	1.92	10	1
1:A:30:ARG:CA	1:A:35:THR:HG21	0.40	2.40	15	1
1:B:123:LEU:CD2	1:B:160:VAL:HG21	0.40	2.46	5	1
1:A:40:LEU:N	1:A:40:LEU:HD13	0.40	2.30	13	1
1:A:40:LEU:HD21	1:A:77:VAL:CG2	0.40	2.43	1	1
1:A:73:LEU:HD23	1:B:89:LEU:O	0.40	2.17	17	1
1:B:156:LEU:HD12	1:B:156:LEU:O	0.40	2.16	12	1
1:A:49:ILE:CD1	1:B:102:LEU:CD2	0.40	3.00	19	1
1:A:34:ALA:CA	1:B:89:LEU:HD21	0.40	2.47	19	1
1:A:23:ILE:HG21	1:B:102:LEU:CD1	0.40	2.47	8	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	72/83 (87%)	68±1 (94±1%)	4±1 (5±1%)	0±1 (1±1%)	33	77
1	B	72/83 (87%)	68±1 (94±1%)	4±1 (5±1%)	0±0 (0±1%)	42	80
All	All	2880/3320 (87%)	2720 (94%)	146 (5%)	14 (0%)	37	78

All 4 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	71	GLY	5
1	B	154	GLY	3
1	A	14	GLU	3
1	B	97	GLU	3

### 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	62/72 (86%)	42±3 (67±5%)	20±3 (33±5%)	1	12
1	B	62/72 (86%)	44±3 (70±5%)	18±3 (30±5%)	2	17
All	All	2480/2880 (86%)	1705 (69%)	775 (31%)	1	15

All 94 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	B	124	HIS	20
1	A	41	HIS	20
1	A	35	THR	19

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Mol	Chain	Res	Type	Models (Total)
1	A	31	THR	18
1	A	21	SER	17
1	A	54	THR	17
1	A	55	GLU	16
1	B	104	SER	16
1	B	138	GLU	16
1	B	118	THR	15
1	A	26	LYS	15
1	A	73	LEU	15
1	B	140	MET	15
1	A	18	ARG	15
1	B	156	LEU	15
1	B	137	THR	14
1	B	155	LYS	14
1	B	109	LYS	13
1	A	72	LYS	13
1	B	101	ARG	12
1	A	33	LEU	12
1	A	5	LEU	12
1	B	114	THR	12
1	A	75	LEU	12
1	A	70	ARG	11
1	A	57	MET	11
1	B	144	ASP	11
1	A	58	SER	11
1	A	28	MET	11
1	B	158	LEU	10
1	A	36	LYS	10
1	A	65	LEU	10
1	B	88	LEU	10
1	B	91	LYS	10
1	A	64	LYS	10
1	A	61	ASP	9
1	B	151	LYS	9
1	B	113	ARG	9
1	A	8	LYS	9
1	B	161	LEU	9
1	B	147	LYS	9
1	B	148	LEU	9
1	A	48	LYS	9
1	A	17	LEU	9
1	A	67	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	B	97	GLU	8
1	B	142	LEU	8
1	B	85	ILE	8
1	B	116	LEU	8
1	A	30	ARG	8
1	B	119	LYS	8
1	A	68	LYS	8
1	A	59	LEU	7
1	A	47	LEU	7
1	A	40	LEU	7
1	B	100	LEU	7
1	A	37	ASP	7
1	B	141	SER	7
1	B	153	ARG	7
1	B	110	GLU	7
1	A	63	ARG	6
1	B	111	MET	6
1	B	150	GLU	5
1	B	120	ASP	5
1	A	60	THR	5
1	A	7	MET	5
1	A	78	LEU	4
1	A	27	GLU	4
1	B	135	THR	4
1	A	14	GLU	4
1	A	2	ILE	4
1	A	74	GLN	4
1	A	50	ASN	3
1	B	131	LYS	3
1	B	133	ASN	3
1	B	146	ARG	3
1	B	90	MET	3
1	B	89	LEU	2
1	B	123	LEU	2
1	B	143	THR	2
1	B	130	LEU	2
1	A	29	THR	2
1	B	112	THR	2
1	B	105	GLN	2
1	B	122	ASN	2
1	A	45	ILE	1
1	A	6	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	106	ILE	1
1	A	19	LEU	1
1	B	102	LEU	1
1	A	39	ASN	1
1	A	69	SER	1
1	B	157	GLN	1
1	B	128	ILE	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