



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:15 PM BST

PDB ID : 1JBJ  
Title : CD3 Epsilon and gamma Ectodomain Fragment Complex in Single-Chain Construct  
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Deposited on : 2001-06-05

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  
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

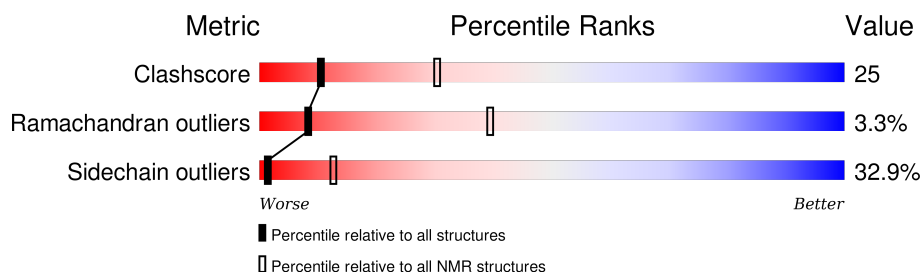
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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	186	<div> <div></div> <div>35%</div> <div>38%</div> <div>6%</div> <div>20%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 18 models. Model 12 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:6-A:80, A:113-A:185 (148)	0.69	12

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 6, 8, 9, 10, 12, 13, 14, 15, 18
2	1, 2, 5, 7, 11, 16, 17

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

There is only 1 type of molecule in this entry. The entry contains 2858 atoms, of which 1411 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CD3 Epsilon and gamma Ectodomain Fragment Complex.

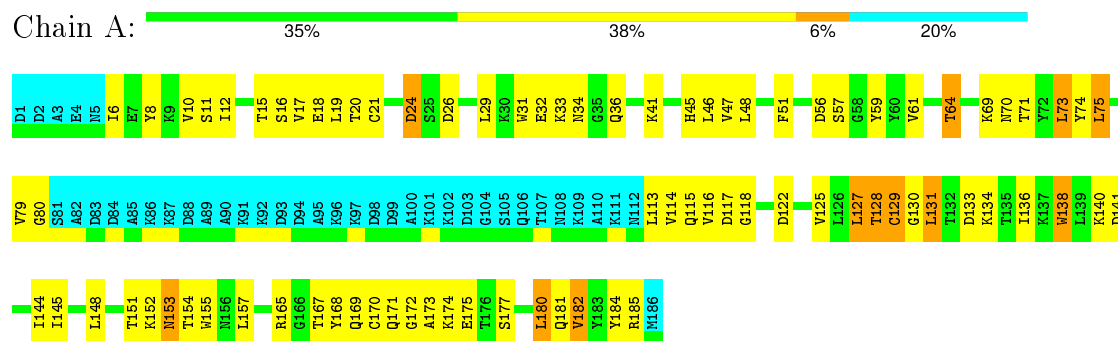
Mol	Chain	Residues	Atoms						Trace
1	A	186	Total	C	H	N	O	S	0
			2858	892	1411	249	301	5	

## 4 Residue-property plots [i](#)

### 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: CD3 Epsilon and gamma Ectodomain Fragment Complex

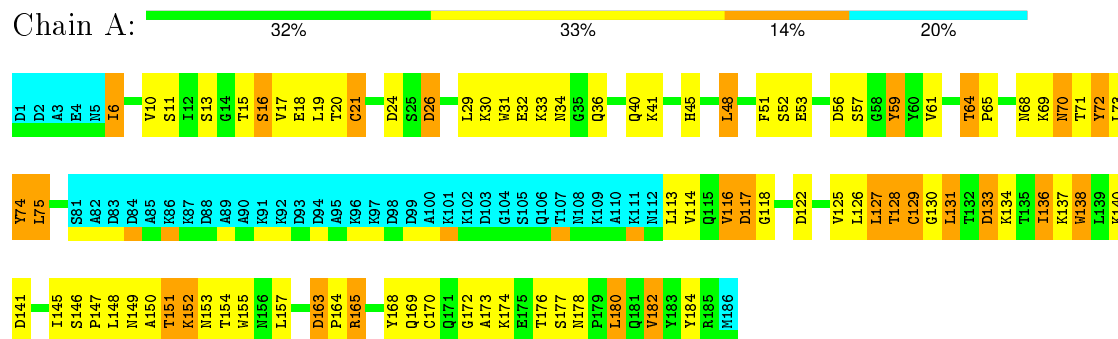


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

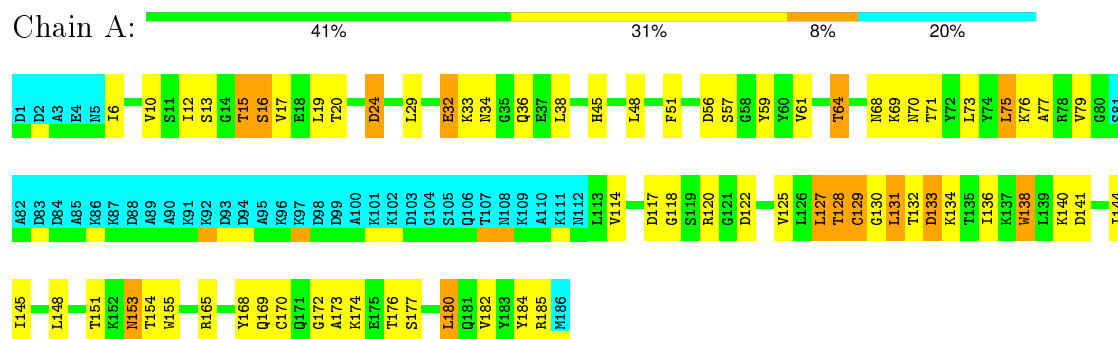
#### 4.2.1 Score per residue for model 1

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



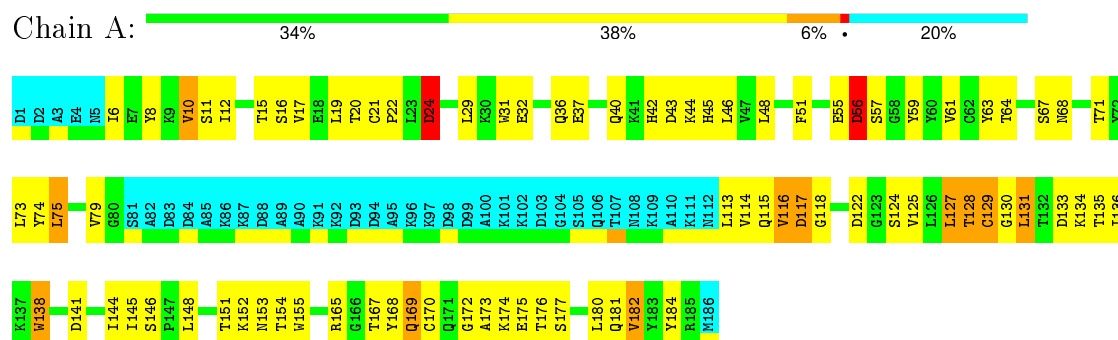
### 4.2.2 Score per residue for model 2

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



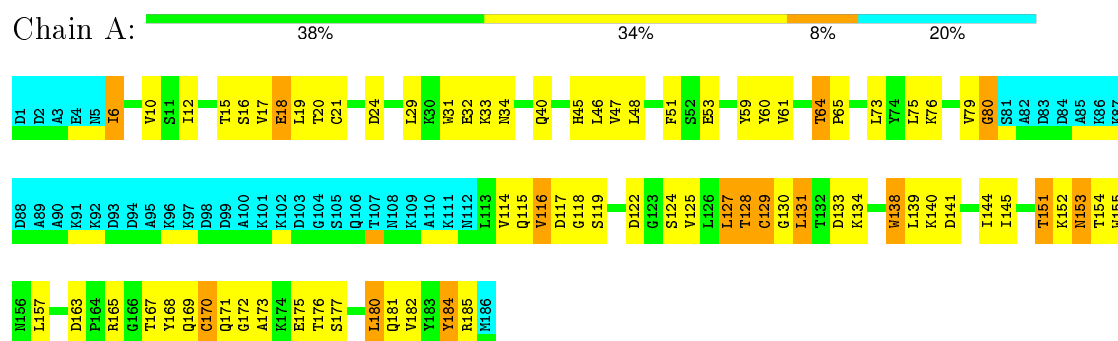
### 4.2.3 Score per residue for model 3

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



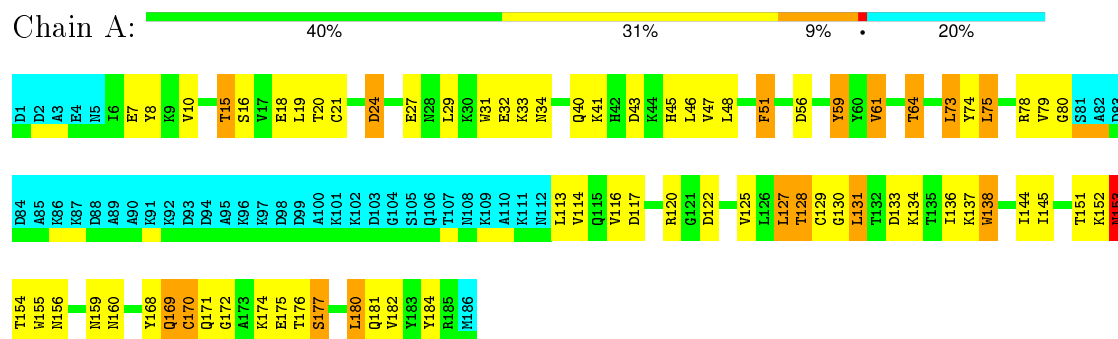
### 4.2.4 Score per residue for model 4

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



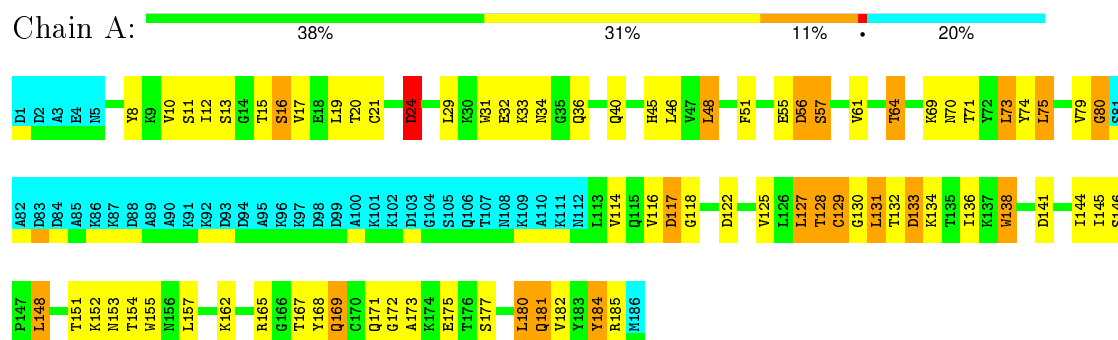
### 4.2.5 Score per residue for model 5

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



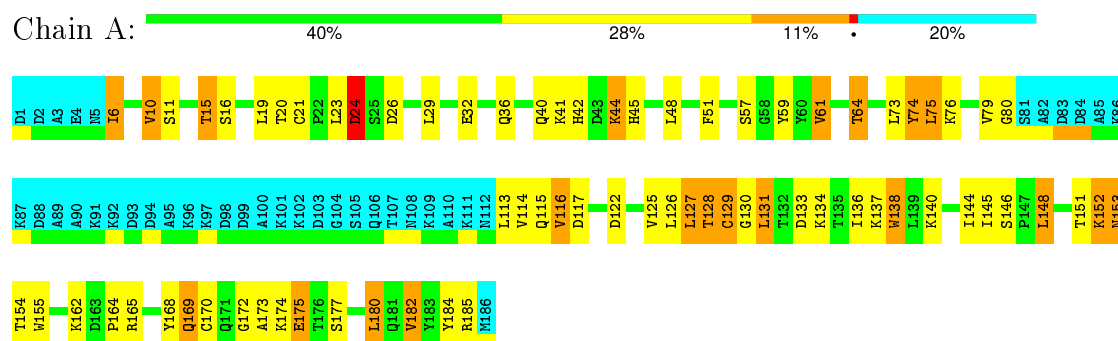
### 4.2.6 Score per residue for model 6

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



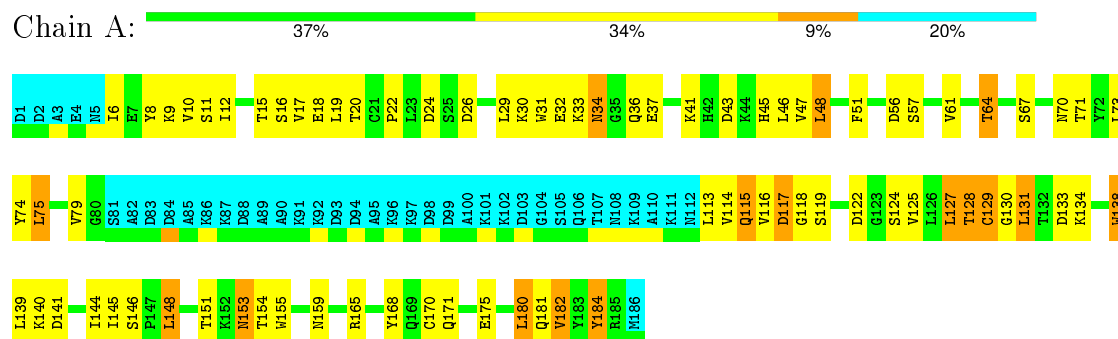
### 4.2.7 Score per residue for model 7

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



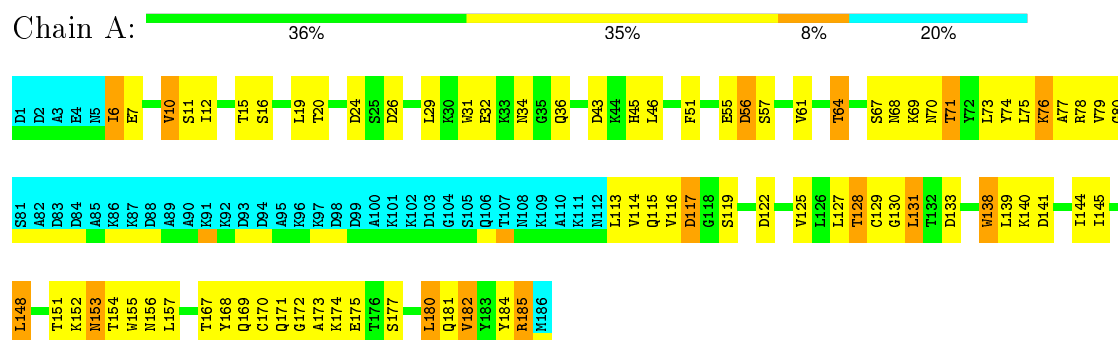
### 4.2.8 Score per residue for model 8

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



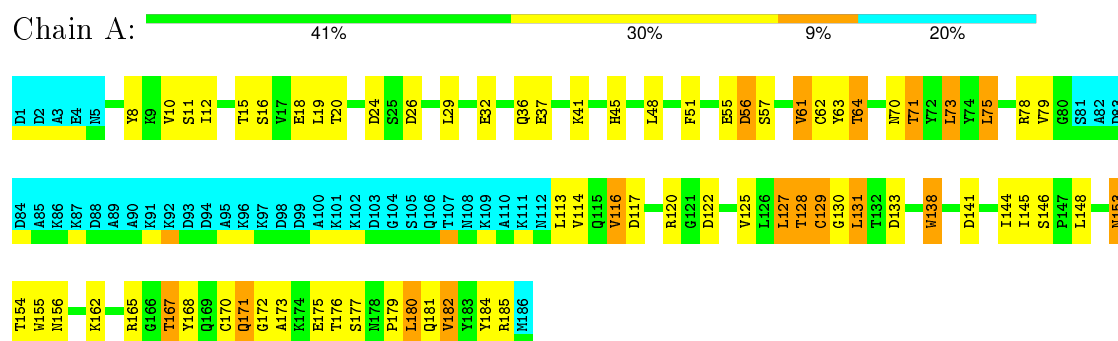
### 4.2.9 Score per residue for model 9

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



### 4.2.10 Score per residue for model 10

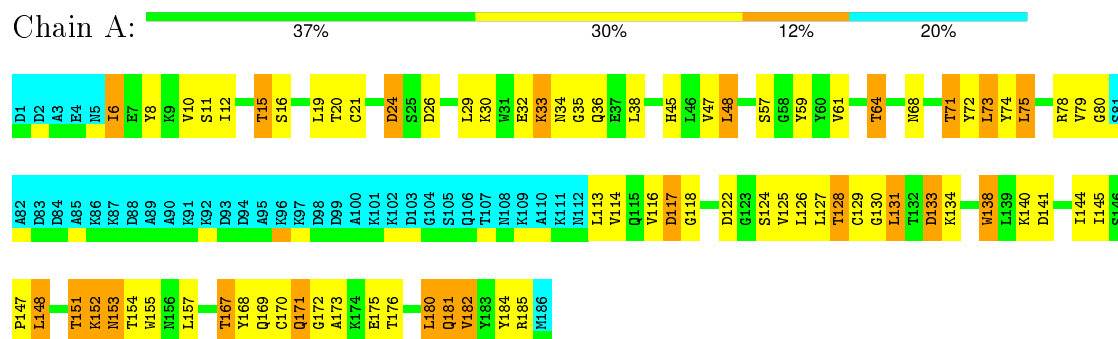
- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex





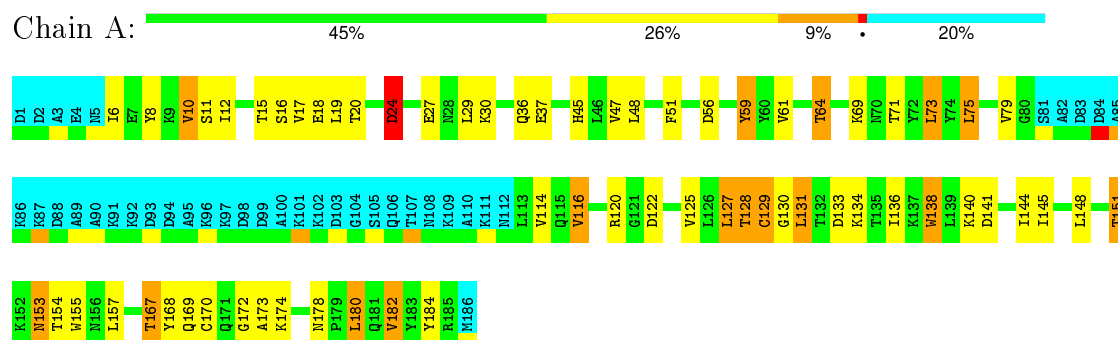
### 4.2.11 Score per residue for model 11

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



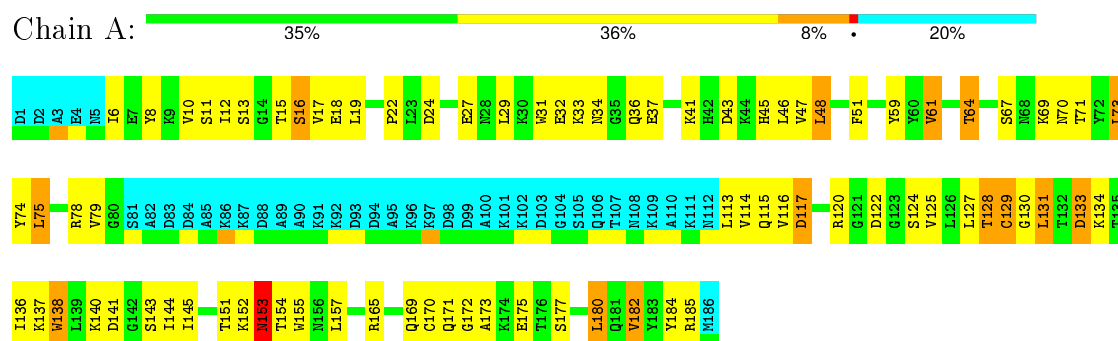
### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



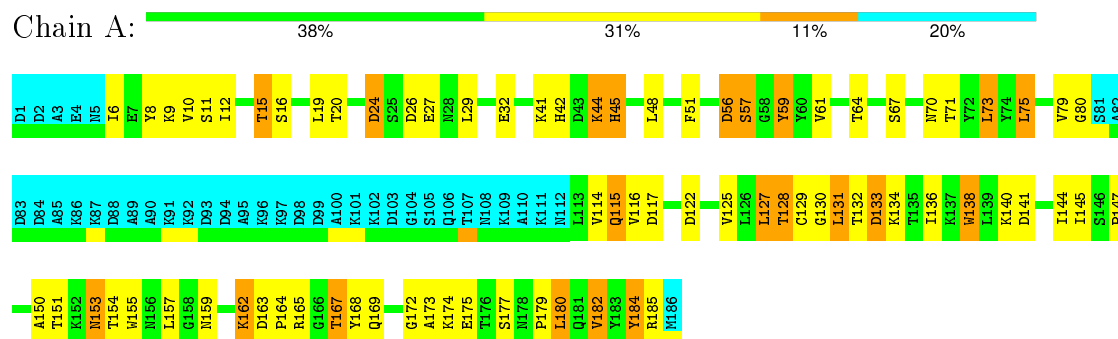
### 4.2.13 Score per residue for model 13

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



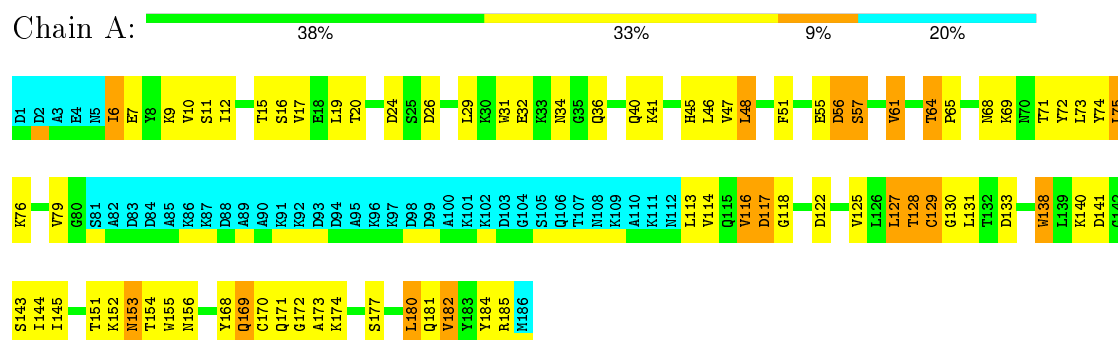
### 4.2.14 Score per residue for model 14

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



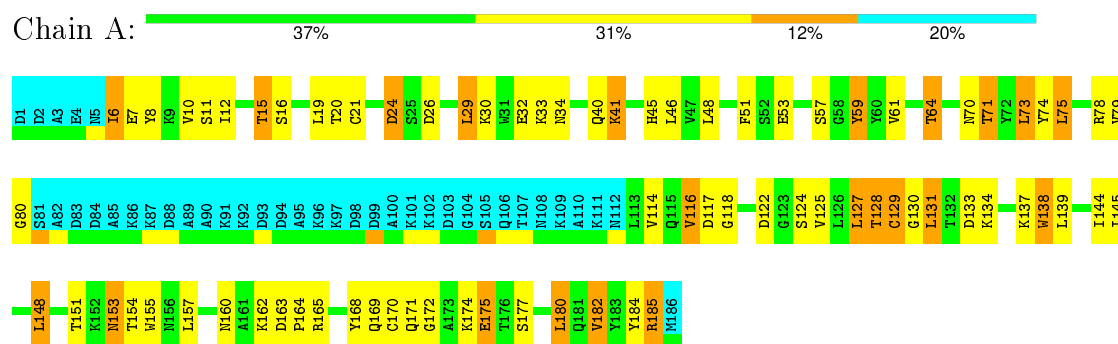
### 4.2.15 Score per residue for model 15

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



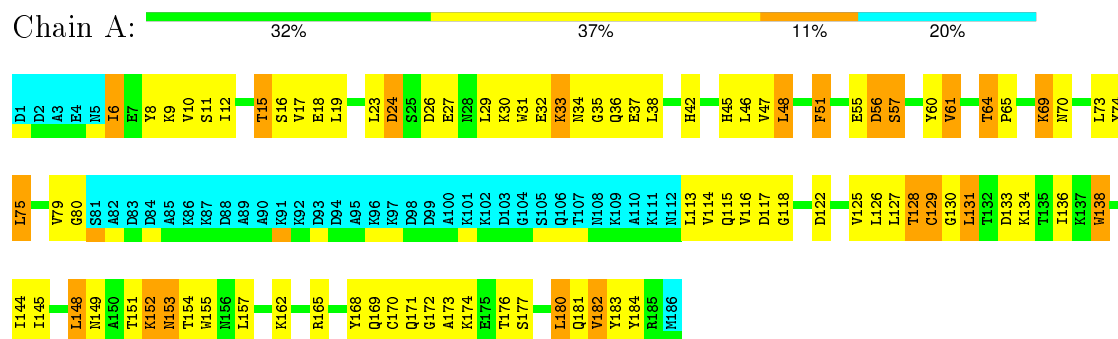
### 4.2.16 Score per residue for model 16

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



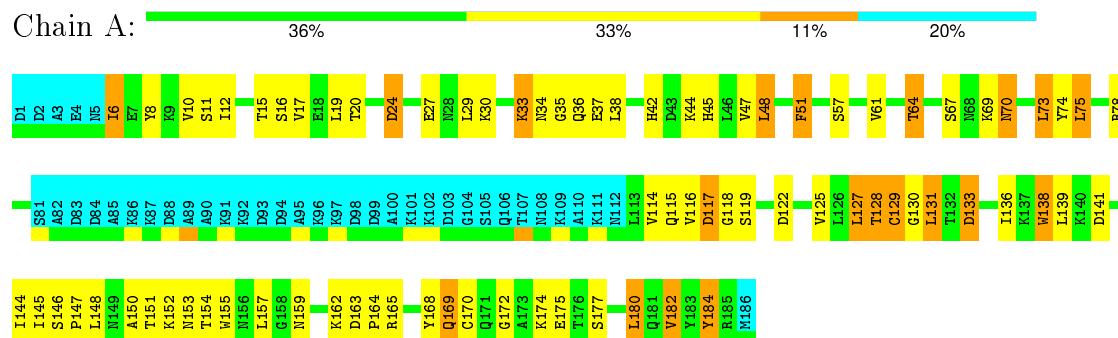
### 4.2.17 Score per residue for model 17

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



### 4.2.18 Score per residue for model 18

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 18 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
DYANA	structure solution	1.4
X-PLOR	structure solution	3.1
X-PLOR	refinement	3.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5072
Number of chemical shift lists	1
Total number of shifts	1754
Number of shifts mapped to atoms	1754
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	1163	1138	1136	56±5
All	All	20934	20484	20448	1017

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD12	1:A:64:THR:HG23	1.00	1.27	4	14
1:A:128:THR:HG23	1:A:154:THR:HG22	0.99	1.34	4	18
1:A:114:VAL:HG11	1:A:180:LEU:HD11	0.98	1.26	5	9
1:A:128:THR:CG2	1:A:154:THR:HG22	0.93	1.93	7	7
1:A:127:LEU:HD21	1:A:180:LEU:HD22	0.88	1.45	2	9
1:A:10:VAL:HG22	1:A:19:LEU:HD22	0.86	1.47	13	4
1:A:10:VAL:HG13	1:A:19:LEU:CD2	0.86	2.01	15	18
1:A:19:LEU:HD11	1:A:48:LEU:HD11	0.86	1.45	6	9
1:A:114:VAL:HG11	1:A:180:LEU:CD1	0.83	2.03	5	7
1:A:116:VAL:HG12	1:A:127:LEU:CD2	0.82	2.05	7	9
1:A:10:VAL:HG13	1:A:19:LEU:HD23	0.82	1.49	7	14
1:A:29:LEU:CD1	1:A:64:THR:HG23	0.82	2.05	4	3
1:A:61:VAL:HG23	1:A:71:THR:O	0.81	1.76	3	10
1:A:180:LEU:HD11	1:A:182:VAL:HG22	0.80	1.52	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:GLU:CB	1:A:61:VAL:HG12	0.80	2.06	5	13
1:A:18:GLU:CG	1:A:47:VAL:HG22	0.79	2.07	17	4
1:A:128:THR:HG23	1:A:154:THR:CG2	0.78	2.09	18	12
1:A:114:VAL:HG11	1:A:180:LEU:CD2	0.77	2.09	8	3
1:A:152:LYS:O	1:A:154:THR:HG23	0.77	1.80	11	6
1:A:116:VAL:HG12	1:A:127:LEU:HD23	0.77	1.56	12	9
1:A:131:LEU:HD12	1:A:133:ASP:HB2	0.77	1.56	11	1
1:A:147:PRO:HG3	1:A:151:THR:HG23	0.76	1.58	1	1
1:A:167:THR:HG23	1:A:181:GLN:HG2	0.75	1.57	11	1
1:A:32:GLU:HB3	1:A:61:VAL:HG12	0.75	1.59	17	12
1:A:135:THR:C	1:A:136:ILE:HD13	0.74	2.02	3	1
1:A:31:TRP:CE3	1:A:46:LEU:HD22	0.74	2.18	17	9
1:A:17:VAL:HG11	1:A:75:LEU:HD11	0.73	1.59	15	3
1:A:136:ILE:HD11	1:A:153:ASN:OD1	0.73	1.82	14	2
1:A:10:VAL:HG13	1:A:19:LEU:HD21	0.72	1.59	8	4
1:A:148:LEU:O	1:A:148:LEU:HD13	0.72	1.84	6	4
1:A:180:LEU:C	1:A:180:LEU:HD12	0.72	2.04	8	1
1:A:114:VAL:HG21	1:A:180:LEU:HD13	0.71	1.61	18	7
1:A:129:CYS:O	1:A:136:ILE:HD13	0.71	1.86	1	4
1:A:148:LEU:HD13	1:A:148:LEU:O	0.71	1.86	8	4
1:A:125:VAL:HG11	1:A:184:TYR:OH	0.71	1.84	3	2
1:A:6:ILE:N	1:A:6:ILE:HD12	0.71	1.99	15	1
1:A:117:ASP:O	1:A:125:VAL:HG13	0.71	1.86	3	17
1:A:125:VAL:HG11	1:A:184:TYR:CE2	0.71	2.20	17	7
1:A:116:VAL:HB	1:A:127:LEU:HD23	0.71	1.61	14	1
1:A:133:ASP:OD1	1:A:173:ALA:HB3	0.70	1.87	10	5
1:A:127:LEU:HD21	1:A:182:VAL:HG11	0.69	1.63	11	5
1:A:128:THR:HG22	1:A:153:ASN:O	0.69	1.86	1	18
1:A:32:GLU:HB2	1:A:61:VAL:HG12	0.69	1.63	1	5
1:A:130:GLY:O	1:A:133:ASP:HB2	0.69	1.88	14	9
1:A:136:ILE:HD12	1:A:153:ASN:HA	0.69	1.61	1	3
1:A:130:GLY:C	1:A:131:LEU:HD23	0.69	2.08	18	6
1:A:125:VAL:HG21	1:A:164:PRO:HG3	0.69	1.63	1	1
1:A:114:VAL:HG21	1:A:180:LEU:CD1	0.68	2.18	18	5
1:A:12:ILE:HD13	1:A:79:VAL:HG12	0.68	1.64	11	2
1:A:131:LEU:HD11	1:A:175:GLU:CB	0.68	2.18	10	4
1:A:64:THR:HG22	1:A:65:PRO:HD2	0.68	1.66	17	4
1:A:157:LEU:HD22	1:A:168:TYR:CZ	0.67	2.25	14	2
1:A:131:LEU:HD11	1:A:175:GLU:CG	0.67	2.20	4	2
1:A:168:TYR:CD1	1:A:182:VAL:HG23	0.67	2.25	8	1
1:A:182:VAL:HG12	1:A:184:TYR:CE1	0.67	2.25	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:THR:HG23	1:A:181:GLN:CG	0.66	2.20	11	1
1:A:131:LEU:HD13	1:A:175:GLU:HB3	0.66	1.67	5	1
1:A:74:TYR:CZ	1:A:116:VAL:HG22	0.66	2.26	16	2
1:A:41:LYS:HE3	1:A:46:LEU:HD12	0.66	1.66	5	2
1:A:41:LYS:HE2	1:A:46:LEU:HD12	0.66	1.65	15	1
1:A:170:CYS:O	1:A:176:THR:HG23	0.66	1.91	2	6
1:A:41:LYS:CE	1:A:46:LEU:HD12	0.65	2.22	16	2
1:A:127:LEU:HD21	1:A:182:VAL:CG1	0.65	2.21	14	1
1:A:74:TYR:CE2	1:A:116:VAL:HG22	0.65	2.27	3	1
1:A:8:TYR:CD2	1:A:73:LEU:HD13	0.65	2.26	6	3
1:A:129:CYS:HB2	1:A:138:TRP:CH2	0.65	2.27	15	11
1:A:10:VAL:CG1	1:A:19:LEU:HD23	0.65	2.22	7	13
1:A:135:THR:O	1:A:136:ILE:HD13	0.65	1.92	3	1
1:A:130:GLY:C	1:A:131:LEU:HD22	0.64	2.13	1	7
1:A:138:TRP:C	1:A:139:LEU:HD12	0.64	2.12	18	2
1:A:130:GLY:HA3	1:A:136:ILE:HD12	0.64	1.68	3	1
1:A:114:VAL:HG11	1:A:180:LEU:HD23	0.63	1.69	8	1
1:A:131:LEU:HD11	1:A:175:GLU:HB2	0.63	1.68	9	4
1:A:157:LEU:HD13	1:A:184:TYR:OH	0.63	1.93	4	3
1:A:29:LEU:HD12	1:A:64:THR:HG22	0.62	1.71	2	2
1:A:18:GLU:HG3	1:A:47:VAL:HG22	0.62	1.69	17	2
1:A:131:LEU:HD11	1:A:175:GLU:HB3	0.61	1.71	18	1
1:A:12:ILE:HG21	1:A:79:VAL:CG1	0.61	2.25	13	3
1:A:114:VAL:HG23	1:A:128:THR:O	0.61	1.94	2	4
1:A:131:LEU:HD13	1:A:175:GLU:HB2	0.61	1.70	11	1
1:A:15:THR:HG23	1:A:80:GLY:O	0.61	1.96	7	4
1:A:18:GLU:HG2	1:A:47:VAL:HG22	0.60	1.73	17	3
1:A:130:GLY:HA2	1:A:136:ILE:HD11	0.60	1.72	2	2
1:A:51:PHE:HB3	1:A:79:VAL:HG22	0.60	1.71	2	8
1:A:145:ILE:HG23	1:A:145:ILE:O	0.60	1.96	9	7
1:A:145:ILE:O	1:A:145:ILE:HG23	0.59	1.97	7	11
1:A:24:ASP:O	1:A:29:LEU:HD13	0.59	1.96	11	8
1:A:128:THR:HG22	1:A:154:THR:HG22	0.59	1.74	7	3
1:A:144:ILE:N	1:A:144:ILE:HD12	0.59	2.12	5	6
1:A:17:VAL:HG21	1:A:51:PHE:CD2	0.59	2.33	18	2
1:A:12:ILE:HG21	1:A:79:VAL:HG12	0.59	1.74	10	10
1:A:26:ASP:OD2	1:A:64:THR:HG21	0.59	1.98	14	1
1:A:127:LEU:HD13	1:A:138:TRP:CZ2	0.58	2.32	7	4
1:A:6:ILE:HD12	1:A:6:ILE:H	0.58	1.58	15	1
1:A:8:TYR:CD2	1:A:73:LEU:HD22	0.58	2.33	16	1
1:A:114:VAL:CG1	1:A:180:LEU:HD11	0.58	2.28	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:VAL:HG21	1:A:163:ASP:OD2	0.58	1.98	16	1
1:A:127:LEU:HD21	1:A:157:LEU:HD11	0.58	1.75	11	4
1:A:130:GLY:O	1:A:132:THR:N	0.58	2.34	6	2
1:A:17:VAL:HB	1:A:48:LEU:HD12	0.57	1.76	1	2
1:A:47:VAL:C	1:A:48:LEU:HD23	0.57	2.20	17	6
1:A:114:VAL:HG13	1:A:128:THR:O	0.57	1.99	14	2
1:A:51:PHE:O	1:A:79:VAL:HG22	0.57	2.00	14	2
1:A:131:LEU:HD13	1:A:175:GLU:CB	0.57	2.28	5	1
1:A:125:VAL:HG22	1:A:160:ASN:OD1	0.57	2.00	16	2
1:A:182:VAL:HG12	1:A:184:TYR:CE2	0.57	2.35	16	6
1:A:48:LEU:HD11	1:A:75:LEU:HD11	0.56	1.77	14	3
1:A:131:LEU:HD21	1:A:175:GLU:HB2	0.56	1.76	4	2
1:A:12:ILE:HD12	1:A:12:ILE:N	0.56	2.15	10	5
1:A:51:PHE:CE2	1:A:75:LEU:HD22	0.56	2.35	17	4
1:A:29:LEU:HD12	1:A:64:THR:CG2	0.56	2.28	9	5
1:A:144:ILE:HD12	1:A:144:ILE:N	0.56	2.16	11	5
1:A:74:TYR:CZ	1:A:116:VAL:HG13	0.56	2.36	8	1
1:A:151:THR:HG23	1:A:151:THR:O	0.56	2.01	3	5
1:A:127:LEU:CD2	1:A:182:VAL:HG11	0.56	2.31	11	1
1:A:167:THR:HG22	1:A:179:PRO:CB	0.56	2.30	10	1
1:A:157:LEU:HD22	1:A:168:TYR:CE2	0.56	2.36	18	1
1:A:127:LEU:CD1	1:A:157:LEU:HD21	0.56	2.30	14	1
1:A:8:TYR:CG	1:A:73:LEU:HD13	0.55	2.35	6	4
1:A:75:LEU:HD22	1:A:76:LYS:N	0.55	2.16	2	2
1:A:10:VAL:HG22	1:A:19:LEU:HD23	0.55	1.77	6	12
1:A:151:THR:O	1:A:151:THR:HG23	0.55	2.01	14	3
1:A:114:VAL:HG22	1:A:129:CYS:SG	0.55	2.42	7	2
1:A:139:LEU:N	1:A:139:LEU:HD12	0.55	2.16	9	1
1:A:157:LEU:HD21	1:A:168:TYR:CE2	0.54	2.37	1	1
1:A:12:ILE:HG21	1:A:79:VAL:HG11	0.54	1.79	13	1
1:A:61:VAL:HG21	1:A:70:ASN:ND2	0.54	2.17	1	2
1:A:139:LEU:HD12	1:A:139:LEU:N	0.54	2.17	18	1
1:A:131:LEU:N	1:A:131:LEU:HD23	0.54	2.17	6	2
1:A:125:VAL:HG11	1:A:184:TYR:CZ	0.54	2.38	13	6
1:A:130:GLY:O	1:A:131:LEU:HG	0.54	2.03	16	6
1:A:114:VAL:HG11	1:A:180:LEU:HD22	0.54	1.80	18	1
1:A:26:ASP:HB2	1:A:64:THR:HG21	0.54	1.80	8	2
1:A:131:LEU:HD11	1:A:175:GLU:HG3	0.54	1.80	10	1
1:A:116:VAL:HG21	1:A:184:TYR:OH	0.53	2.03	12	1
1:A:153:ASN:ND2	1:A:153:ASN:O	0.53	2.41	14	1
1:A:182:VAL:HG12	1:A:184:TYR:HE1	0.53	1.63	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:TRP:CE3	1:A:155:TRP:HB2	0.53	2.38	13	17
1:A:131:LEU:HD23	1:A:175:GLU:HB3	0.53	1.81	8	2
1:A:116:VAL:HG12	1:A:127:LEU:HD21	0.53	1.78	3	2
1:A:12:ILE:HG13	1:A:17:VAL:HG22	0.53	1.80	18	6
1:A:127:LEU:HD11	1:A:157:LEU:HD21	0.52	1.81	14	1
1:A:115:GLN:O	1:A:128:THR:OG1	0.52	2.24	18	5
1:A:19:LEU:HD21	1:A:75:LEU:HD11	0.52	1.80	13	2
1:A:140:LYS:HD3	1:A:145:ILE:HD12	0.52	1.80	13	1
1:A:51:PHE:CZ	1:A:75:LEU:HD22	0.52	2.39	13	5
1:A:138:TRP:CZ3	1:A:155:TRP:HB2	0.52	2.39	10	10
1:A:131:LEU:HD23	1:A:175:GLU:CB	0.52	2.35	8	2
1:A:12:ILE:HD13	1:A:79:VAL:CG1	0.52	2.34	9	3
1:A:10:VAL:HG22	1:A:19:LEU:CD2	0.51	2.34	1	1
1:A:8:TYR:CE2	1:A:71:THR:HG21	0.51	2.40	8	1
1:A:59:TYR:CE2	1:A:74:TYR:CE2	0.51	2.99	1	2
1:A:6:ILE:HD13	1:A:6:ILE:N	0.51	2.21	11	3
1:A:12:ILE:CG1	1:A:17:VAL:HG22	0.51	2.35	13	1
1:A:59:TYR:N	1:A:59:TYR:CD1	0.51	2.77	14	3
1:A:131:LEU:HG	1:A:131:LEU:O	0.51	2.05	2	2
1:A:15:THR:HG22	1:A:79:VAL:CG2	0.51	2.36	17	2
1:A:125:VAL:HG21	1:A:184:TYR:CD2	0.51	2.41	11	1
1:A:74:TYR:CZ	1:A:116:VAL:CG2	0.51	2.94	9	5
1:A:19:LEU:HD21	1:A:75:LEU:CD1	0.51	2.35	10	5
1:A:6:ILE:HG22	1:A:7:GLU:H	0.51	1.65	15	1
1:A:172:GLY:N	1:A:175:GLU:O	0.51	2.44	18	5
1:A:180:LEU:CD1	1:A:182:VAL:HG22	0.51	2.30	8	1
1:A:75:LEU:HD23	1:A:76:LYS:N	0.51	2.21	9	1
1:A:163:ASP:N	1:A:164:PRO:CD	0.50	2.74	14	2
1:A:23:LEU:HD11	1:A:69:LYS:HB2	0.50	1.83	17	1
1:A:19:LEU:HD11	1:A:75:LEU:CD1	0.50	2.36	11	2
1:A:75:LEU:HD22	1:A:75:LEU:C	0.50	2.27	2	1
1:A:15:THR:HG22	1:A:79:VAL:HG23	0.50	1.83	17	3
1:A:73:LEU:C	1:A:73:LEU:HD12	0.50	2.27	9	1
1:A:125:VAL:CG1	1:A:157:LEU:HD12	0.49	2.37	12	2
1:A:48:LEU:HD11	1:A:75:LEU:CD1	0.49	2.37	5	5
1:A:48:LEU:HD13	1:A:51:PHE:CE1	0.49	2.42	1	2
1:A:64:THR:HG22	1:A:65:PRO:CD	0.49	2.37	1	2
1:A:8:TYR:OH	1:A:71:THR:HG21	0.49	2.08	8	1
1:A:59:TYR:CD1	1:A:59:TYR:N	0.49	2.80	12	1
1:A:127:LEU:O	1:A:155:TRP:N	0.49	2.46	8	17
1:A:113:LEU:CB	1:A:131:LEU:HD12	0.49	2.37	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:N	1:A:6:ILE:CD1	0.49	2.71	15	1
1:A:61:VAL:O	1:A:61:VAL:HG13	0.49	2.08	3	1
1:A:127:LEU:HB2	1:A:138:TRP:CH2	0.48	2.43	13	3
1:A:182:VAL:HG12	1:A:184:TYR:CZ	0.48	2.42	13	4
1:A:149:ASN:O	1:A:150:ALA:HB3	0.48	2.09	1	1
1:A:129:CYS:CB	1:A:138:TRP:CH2	0.48	2.96	5	1
1:A:157:LEU:HD22	1:A:184:TYR:OH	0.48	2.08	6	1
1:A:75:LEU:C	1:A:75:LEU:HD22	0.48	2.28	7	1
1:A:128:THR:CG2	1:A:154:THR:CG2	0.48	2.91	8	12
1:A:74:TYR:CE1	1:A:116:VAL:HG22	0.48	2.43	7	1
1:A:145:ILE:O	1:A:155:TRP:CH2	0.48	2.66	1	2
1:A:168:TYR:CD1	1:A:168:TYR:N	0.48	2.81	10	8
1:A:55:GLU:O	1:A:56:ASP:CB	0.48	2.62	17	6
1:A:167:THR:HG22	1:A:181:GLN:OE1	0.48	2.09	6	1
1:A:74:TYR:CE2	1:A:116:VAL:CG2	0.47	2.97	3	1
1:A:10:VAL:CG2	1:A:19:LEU:HD22	0.47	2.32	17	2
1:A:74:TYR:CZ	1:A:116:VAL:CG1	0.47	2.98	8	1
1:A:163:ASP:CB	1:A:164:PRO:CD	0.47	2.92	1	1
1:A:17:VAL:O	1:A:48:LEU:N	0.47	2.46	1	2
1:A:125:VAL:CG1	1:A:184:TYR:CE2	0.47	2.97	2	2
1:A:74:TYR:CE2	1:A:116:VAL:CG1	0.47	2.98	18	3
1:A:180:LEU:C	1:A:180:LEU:CD1	0.47	2.77	8	1
1:A:8:TYR:CB	1:A:73:LEU:HD21	0.47	2.40	13	1
1:A:32:GLU:OE2	1:A:61:VAL:HG11	0.47	2.09	8	1
1:A:51:PHE:HE2	1:A:75:LEU:HD22	0.47	1.70	17	1
1:A:57:SER:CB	1:A:74:TYR:CZ	0.47	2.98	3	2
1:A:159:ASN:O	1:A:163:ASP:N	0.47	2.40	14	1
1:A:125:VAL:HG11	1:A:184:TYR:HH	0.47	1.70	3	1
1:A:116:VAL:CG1	1:A:180:LEU:HD21	0.47	2.40	9	1
1:A:168:TYR:N	1:A:168:TYR:CD1	0.47	2.82	2	3
1:A:145:ILE:O	1:A:145:ILE:CG2	0.46	2.63	11	9
1:A:74:TYR:OH	1:A:116:VAL:HG22	0.46	2.10	15	1
1:A:148:LEU:CD1	1:A:148:LEU:O	0.46	2.63	16	2
1:A:15:THR:O	1:A:79:VAL:HG21	0.46	2.09	2	1
1:A:12:ILE:HG23	1:A:16:SER:O	0.46	2.10	2	1
1:A:73:LEU:HD12	1:A:73:LEU:C	0.46	2.30	10	1
1:A:131:LEU:HD13	1:A:131:LEU:N	0.46	2.25	1	1
1:A:168:TYR:CE2	1:A:182:VAL:CG2	0.46	2.99	1	3
1:A:125:VAL:HG12	1:A:157:LEU:HD12	0.46	1.87	16	3
1:A:19:LEU:CD1	1:A:48:LEU:HD11	0.46	2.32	6	1
1:A:116:VAL:CB	1:A:127:LEU:HD23	0.46	2.37	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:THR:HA	1:A:153:ASN:O	0.46	2.10	14	8
1:A:131:LEU:N	1:A:131:LEU:CD2	0.46	2.79	2	2
1:A:145:ILE:CG2	1:A:145:ILE:O	0.46	2.63	9	5
1:A:130:GLY:HA3	1:A:136:ILE:CD1	0.46	2.40	18	2
1:A:171:GLN:CG	1:A:176:THR:HG23	0.45	2.41	17	1
1:A:131:LEU:H	1:A:131:LEU:CD2	0.45	2.23	6	2
1:A:6:ILE:N	1:A:6:ILE:HD13	0.45	2.26	9	3
1:A:182:VAL:CG1	1:A:184:TYR:CE2	0.45	2.98	16	3
1:A:127:LEU:HD11	1:A:182:VAL:HG21	0.45	1.87	17	2
1:A:19:LEU:HD11	1:A:75:LEU:HD12	0.45	1.89	18	4
1:A:59:TYR:CE2	1:A:74:TYR:CD2	0.45	3.05	1	1
1:A:168:TYR:CD2	1:A:182:VAL:HG21	0.45	2.46	7	2
1:A:172:GLY:O	1:A:173:ALA:C	0.45	2.55	15	12
1:A:127:LEU:HD21	1:A:157:LEU:CD1	0.45	2.42	11	4
1:A:8:TYR:CD1	1:A:73:LEU:CD2	0.45	3.00	18	1
1:A:168:TYR:CD2	1:A:182:VAL:CG2	0.45	2.99	12	3
1:A:114:VAL:CG1	1:A:180:LEU:CD1	0.45	2.95	2	1
1:A:171:GLN:HG3	1:A:176:THR:HG23	0.45	1.89	11	1
1:A:138:TRP:CZ2	1:A:170:CYS:SG	0.45	3.10	3	1
1:A:127:LEU:CB	1:A:138:TRP:CH2	0.45	3.00	9	2
1:A:131:LEU:C	1:A:132:THR:HG23	0.45	2.32	14	1
1:A:127:LEU:O	1:A:138:TRP:CZ3	0.45	2.70	15	8
1:A:131:LEU:N	1:A:131:LEU:HD13	0.45	2.26	12	5
1:A:61:VAL:HG22	1:A:70:ASN:HB2	0.44	1.90	1	1
1:A:12:ILE:CG2	1:A:79:VAL:HG12	0.44	2.42	11	1
1:A:12:ILE:HD11	1:A:77:ALA:HB1	0.44	1.88	9	1
1:A:33:LYS:O	1:A:35:GLY:N	0.44	2.51	18	3
1:A:114:VAL:HG11	1:A:180:LEU:HD21	0.44	1.90	14	1
1:A:157:LEU:CD2	1:A:168:TYR:CZ	0.44	2.99	14	1
1:A:33:LYS:CB	1:A:60:TYR:CE2	0.44	3.01	17	1
1:A:144:ILE:N	1:A:144:ILE:CD1	0.44	2.81	5	2
1:A:21:CYS:CB	1:A:44:LYS:O	0.43	2.66	7	2
1:A:138:TRP:O	1:A:139:LEU:HD12	0.43	2.13	4	1
1:A:167:THR:HG22	1:A:179:PRO:HB3	0.43	1.89	10	2
1:A:19:LEU:HD12	1:A:46:LEU:HD23	0.43	1.89	5	1
1:A:131:LEU:HD21	1:A:175:GLU:CB	0.43	2.43	10	1
1:A:126:LEU:HD22	1:A:154:THR:OG1	0.43	2.13	1	1
1:A:139:LEU:HD11	1:A:144:ILE:HG13	0.43	1.90	4	1
1:A:126:LEU:HD22	1:A:154:THR:CB	0.43	2.43	1	1
1:A:127:LEU:HD11	1:A:157:LEU:HD11	0.43	1.89	9	2
1:A:21:CYS:HB2	1:A:31:TRP:CZ2	0.43	2.48	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:VAL:CG2	1:A:125:VAL:CG1	0.43	2.97	18	1
1:A:182:VAL:HG12	1:A:184:TYR:OH	0.43	2.13	7	1
1:A:139:LEU:HG	1:A:144:ILE:HD13	0.43	1.90	18	2
1:A:147:PRO:HG2	1:A:150:ALA:O	0.43	2.14	14	1
1:A:131:LEU:H	1:A:131:LEU:HD23	0.43	1.72	6	1
1:A:127:LEU:HD21	1:A:180:LEU:CD2	0.43	2.42	18	3
1:A:144:ILE:H	1:A:144:ILE:HD12	0.43	1.74	8	1
1:A:29:LEU:HA	1:A:64:THR:HG23	0.43	1.91	16	1
1:A:147:PRO:CG	1:A:150:ALA:O	0.43	2.67	18	1
1:A:52:SER:O	1:A:56:ASP:N	0.43	2.52	1	1
1:A:152:LYS:O	1:A:153:ASN:HB3	0.42	2.13	1	1
1:A:138:TRP:CD1	1:A:169:GLN:O	0.42	2.72	18	7
1:A:168:TYR:CD1	1:A:182:VAL:CG2	0.42	3.00	8	1
1:A:48:LEU:CD1	1:A:75:LEU:CD1	0.42	2.97	3	3
1:A:127:LEU:HD22	1:A:138:TRP:CZ2	0.42	2.49	3	1
1:A:8:TYR:CG	1:A:73:LEU:HD22	0.42	2.49	5	1
1:A:13:SER:N	1:A:16:SER:O	0.42	2.50	2	4
1:A:131:LEU:CD1	1:A:175:GLU:CB	0.42	2.97	5	1
1:A:61:VAL:HG21	1:A:70:ASN:HB2	0.42	1.90	16	1
1:A:168:TYR:CE2	1:A:182:VAL:HG21	0.42	2.49	12	2
1:A:125:VAL:O	1:A:126:LEU:HD12	0.42	2.14	17	1
1:A:148:LEU:O	1:A:148:LEU:CD1	0.42	2.65	17	1
1:A:8:TYR:CG	1:A:73:LEU:HD21	0.42	2.50	13	1
1:A:147:PRO:HD3	1:A:155:TRP:CZ3	0.42	2.50	11	1
1:A:130:GLY:CA	1:A:136:ILE:HD13	0.42	2.44	5	1
1:A:78:ARG:CG	1:A:79:VAL:N	0.42	2.83	5	3
1:A:113:LEU:O	1:A:131:LEU:HD12	0.42	2.15	17	1
1:A:171:GLN:HG2	1:A:176:THR:HG23	0.42	1.90	17	1
1:A:144:ILE:HD12	1:A:144:ILE:H	0.42	1.74	14	4
1:A:32:GLU:CB	1:A:61:VAL:CG1	0.42	2.98	3	1
1:A:9:LYS:O	1:A:19:LEU:HA	0.42	2.15	17	1
1:A:48:LEU:CD1	1:A:75:LEU:HD11	0.42	2.45	12	1
1:A:44:LYS:CG	1:A:45:HIS:CD2	0.42	3.03	14	1
1:A:32:GLU:O	1:A:61:VAL:HG12	0.42	2.14	14	1
1:A:115:GLN:C	1:A:128:THR:HG1	0.41	2.17	13	1
1:A:12:ILE:N	1:A:12:ILE:CD1	0.41	2.83	6	2
1:A:138:TRP:CE2	1:A:170:CYS:SG	0.41	3.14	18	1
1:A:184:TYR:CD1	1:A:184:TYR:N	0.41	2.88	18	1
1:A:33:LYS:HB3	1:A:60:TYR:CE2	0.41	2.50	17	1
1:A:79:VAL:O	1:A:80:GLY:C	0.41	2.59	6	2
1:A:138:TRP:CD1	1:A:168:TYR:HB3	0.41	2.50	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:VAL:CG2	1:A:19:LEU:HD23	0.41	2.46	6	1
1:A:129:CYS:O	1:A:136:ILE:HD12	0.41	2.14	6	1
1:A:8:TYR:CZ	1:A:22:PRO:HD3	0.41	2.51	8	2
1:A:159:ASN:O	1:A:162:LYS:N	0.41	2.52	18	2
1:A:15:THR:CG2	1:A:80:GLY:O	0.41	2.69	14	1
1:A:163:ASP:N	1:A:164:PRO:HD3	0.41	2.30	14	1
1:A:51:PHE:CZ	1:A:75:LEU:HD13	0.41	2.50	6	1
1:A:10:VAL:CG1	1:A:19:LEU:CD2	0.41	2.95	7	2
1:A:157:LEU:CD2	1:A:168:TYR:CE2	0.41	3.04	1	1
1:A:163:ASP:OD1	1:A:184:TYR:CD1	0.41	2.74	4	1
1:A:8:TYR:CE2	1:A:22:PRO:CD	0.41	3.04	3	1
1:A:136:ILE:CD1	1:A:153:ASN:OD1	0.41	2.69	1	1
1:A:129:CYS:O	1:A:136:ILE:CD1	0.41	2.69	18	1
1:A:152:LYS:O	1:A:153:ASN:ND2	0.41	2.54	7	1
1:A:12:ILE:HA	1:A:16:SER:O	0.41	2.16	2	1
1:A:171:GLN:HA	1:A:176:THR:HG23	0.41	1.92	10	1
1:A:144:ILE:CD1	1:A:144:ILE:N	0.40	2.84	15	2
1:A:167:THR:O	1:A:168:TYR:CD1	0.40	2.74	12	1
1:A:130:GLY:CA	1:A:136:ILE:CD1	0.40	2.99	5	1
1:A:74:TYR:CE2	1:A:116:VAL:HG11	0.40	2.51	18	1
1:A:127:LEU:CG	1:A:157:LEU:HD11	0.40	2.46	9	1
1:A:12:ILE:CD1	1:A:12:ILE:N	0.40	2.84	3	1
1:A:51:PHE:CE2	1:A:77:ALA:O	0.40	2.74	2	1
1:A:130:GLY:HA3	1:A:136:ILE:HD13	0.40	1.92	5	1
1:A:130:GLY:O	1:A:133:ASP:CB	0.40	2.70	10	1
1:A:17:VAL:CB	1:A:48:LEU:HD12	0.40	2.45	6	1
1:A:151:THR:O	1:A:153:ASN:N	0.40	2.51	1	1
1:A:6:ILE:CD1	1:A:6:ILE:N	0.40	2.84	18	1
1:A:33:LYS:CG	1:A:60:TYR:CE1	0.40	3.04	4	1
1:A:8:TYR:CD2	1:A:73:LEU:CD2	0.40	3.04	10	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	148/186 (80%)	122±3 (83±2%)	21±4 (14±2%)	5±1 (3±1%)	8	39
All	All	2664/3348 (80%)	2203 (83%)	374 (14%)	87 (3%)	8	39

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	34	ASN	12
1	A	24	ASP	11
1	A	118	GLY	11
1	A	56	ASP	10
1	A	151	THR	9
1	A	57	SER	9
1	A	80	GLY	5
1	A	185	ARG	4
1	A	113	LEU	3
1	A	165	ARG	3
1	A	164	PRO	2
1	A	131	LEU	2
1	A	153	ASN	2
1	A	129	CYS	1
1	A	59	TYR	1
1	A	68	ASN	1
1	A	163	ASP	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	131/160 (82%)	88±4 (67±3%)	43±4 (33±3%)	1	12
All	All	2358/2880 (82%)	1582 (67%)	776 (33%)	1	12

All 96 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	122	ASP	18

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Mol	Chain	Res	Type	Models (Total)
1	A	45	HIS	18
1	A	128	THR	18
1	A	182	VAL	18
1	A	180	LEU	18
1	A	16	SER	18
1	A	138	TRP	18
1	A	15	THR	18
1	A	75	LEU	17
1	A	64	THR	17
1	A	73	LEU	17
1	A	20	THR	16
1	A	131	LEU	16
1	A	129	CYS	16
1	A	177	SER	15
1	A	169	GLN	15
1	A	11	SER	15
1	A	24	ASP	14
1	A	134	LYS	14
1	A	36	GLN	14
1	A	127	LEU	14
1	A	6	ILE	14
1	A	153	ASN	14
1	A	141	ASP	14
1	A	174	LYS	12
1	A	148	LEU	12
1	A	170	CYS	11
1	A	165	ARG	11
1	A	133	ASP	11
1	A	181	GLN	10
1	A	171	GLN	10
1	A	140	LYS	10
1	A	70	ASN	10
1	A	33	LYS	10
1	A	59	TYR	10
1	A	185	ARG	9
1	A	117	ASP	9
1	A	152	LYS	9
1	A	69	LYS	9
1	A	48	LEU	9
1	A	26	ASP	8
1	A	40	GLN	8
1	A	116	VAL	8

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Mol	Chain	Res	Type	Models (Total)
1	A	71	THR	7
1	A	146	SER	7
1	A	167	THR	7
1	A	30	LYS	7
1	A	41	LYS	7
1	A	57	SER	7
1	A	37	GLU	7
1	A	113	LEU	6
1	A	67	SER	6
1	A	162	LYS	6
1	A	124	SER	6
1	A	61	VAL	6
1	A	27	GLU	6
1	A	43	ASP	5
1	A	184	TYR	5
1	A	120	ARG	5
1	A	42	HIS	5
1	A	21	CYS	5
1	A	68	ASN	5
1	A	115	GLN	5
1	A	137	LYS	5
1	A	156	ASN	4
1	A	51	PHE	4
1	A	78	ARG	4
1	A	119	SER	4
1	A	10	VAL	4
1	A	38	LEU	4
1	A	18	GLU	4
1	A	72	TYR	3
1	A	56	ASP	3
1	A	53	GLU	3
1	A	151	THR	3
1	A	7	GLU	3
1	A	76	LYS	3
1	A	175	GLU	3
1	A	44	LYS	3
1	A	9	LYS	3
1	A	178	ASN	2
1	A	74	TYR	2
1	A	126	LEU	2
1	A	143	SER	2
1	A	63	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	139	LEU	2
1	A	159	ASN	2
1	A	34	ASN	2
1	A	62	CYS	1
1	A	23	LEU	1
1	A	136	ILE	1
1	A	183	TYR	1
1	A	149	ASN	1
1	A	29	LEU	1
1	A	32	GLU	1
1	A	8	TYR	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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 70% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5072

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1754
Number of shifts mapped to atoms	1754
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	157	$0.77 \pm 0.10$	Should be applied
$^{13}\text{C}_\beta$	145	$1.05 \pm 0.10$	Should be applied
$^{13}\text{C}'$	155	$0.46 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	147	$-0.14 \pm 0.37$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1449 atoms were assigned a chemical shift out of a possible 1788. 26 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	698/728 (96%)	278/290 (96%)	286/296 (97%)	134/142 (94%)
Sidechain	689/927 (74%)	452/542 (83%)	228/343 (66%)	9/42 (21%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	62/133 (47%)	60/67 (90%)	0/59 (0%)	2/7 (29%)
Overall	1449/1788 (81%)	790/899 (88%)	514/698 (74%)	145/191 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1557 atoms were assigned a chemical shift out of a possible 2220. 26 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	763/918 (83%)	304/366 (83%)	312/372 (84%)	147/180 (82%)
Sidechain	732/1169 (63%)	479/683 (70%)	242/430 (56%)	11/56 (20%)
Aromatic	62/133 (47%)	60/67 (90%)	0/59 (0%)	2/7 (29%)
Overall	1557/2220 (70%)	843/1116 (76%)	554/861 (64%)	160/243 (66%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	155	TRP	HB2	0.88	4.94 – 1.44	-6.6

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

