



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 03:32 AM BST

PDB ID : 2MQE  
Title : Solution structure of Escherichia coli Outer membrane protein A C-terminal domain  
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Deposited on : 2014-06-19

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

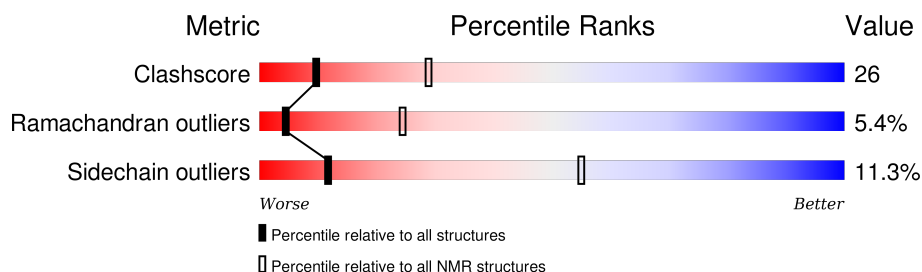
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 15%.

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	

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:190-A:317 (128)	0.28	14

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 24, 25, 27, 29, 30
2	3, 10, 26
3	6, 23
Single-model clusters	28

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

There is only 1 type of molecule in this entry. The entry contains 2212 atoms, of which 1109 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called OmpA domain protein transmembrane region-containing protein.

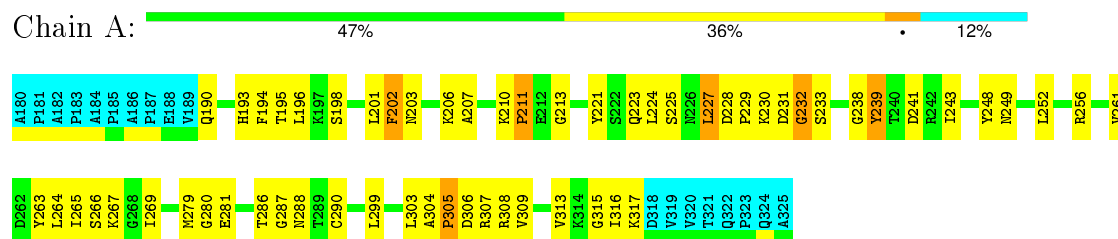
Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	0
			2212	685	1109	195	220	3	

## 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: OmpA domain protein transmembrane region-containing protein

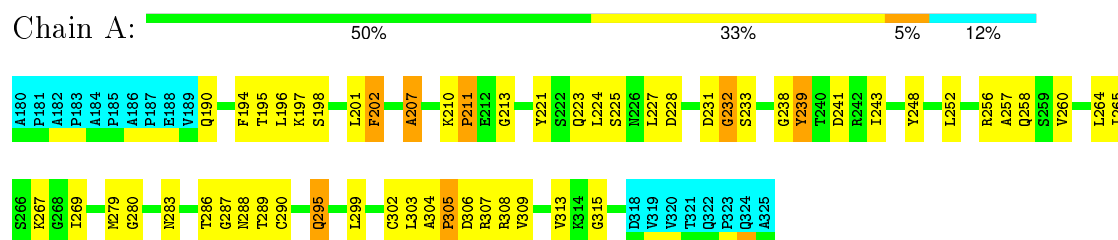


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: OmpA domain protein transmembrane region-containing protein

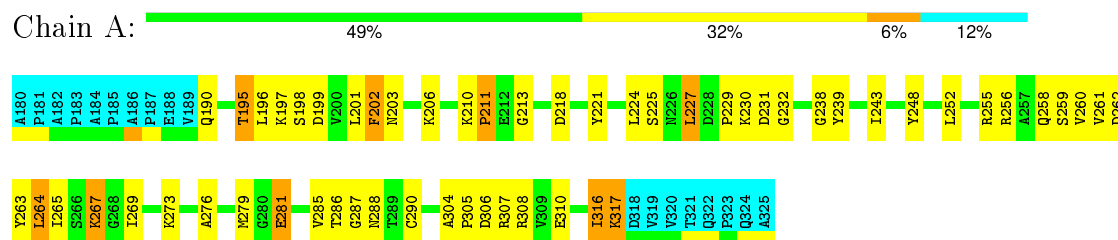


#### 4.2.2 Score per residue for model 2

- Molecule 1: OmpA domain protein transmembrane region-containing protein

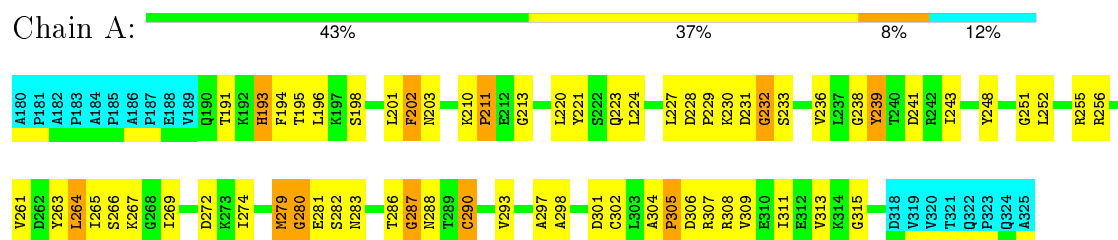






#### 4.2.7 Score per residue for model 7

- Molecule 1: OmpA domain protein transmembrane region-containing protein



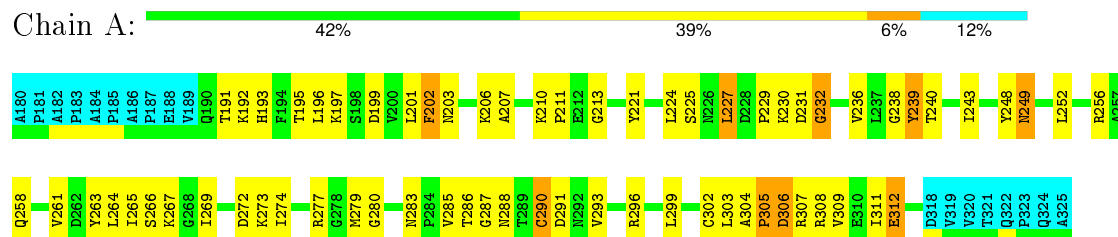
#### 4.2.8 Score per residue for model 8

- Molecule 1: OmpA domain protein transmembrane region-containing protein



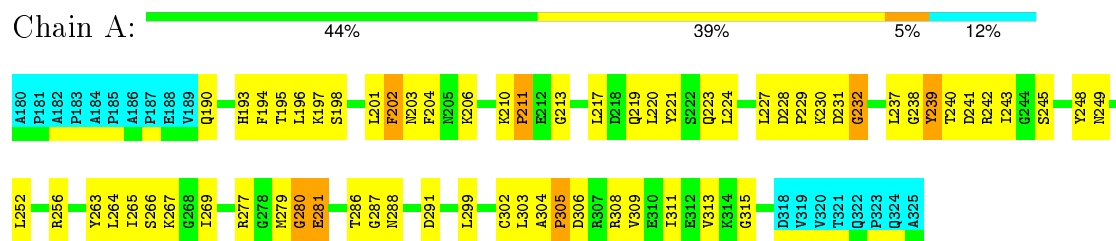
#### 4.2.9 Score per residue for model 9

- Molecule 1: OmpA domain protein transmembrane region-containing protein



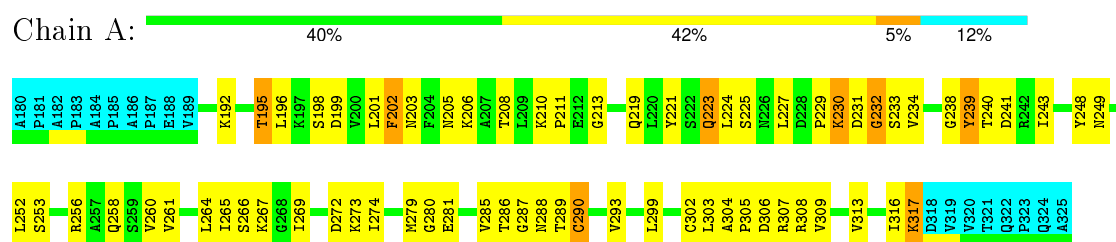
### 4.2.10 Score per residue for model 10

- Molecule 1: OmpA domain protein transmembrane region-containing protein



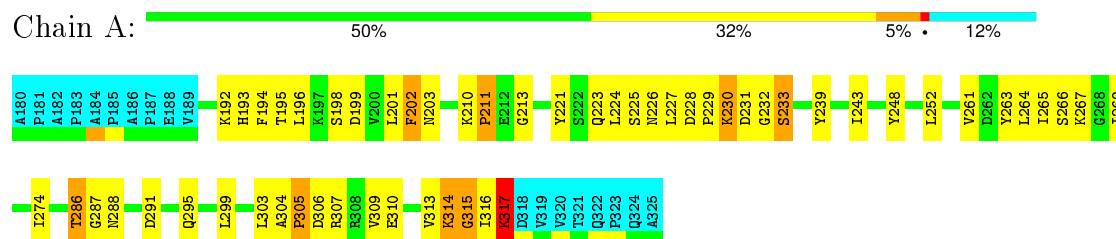
### 4.2.11 Score per residue for model 11

- Molecule 1: OmpA domain protein transmembrane region-containing protein



### 4.2.12 Score per residue for model 12

- Molecule 1: OmpA domain protein transmembrane region-containing protein



### 4.2.13 Score per residue for model 13

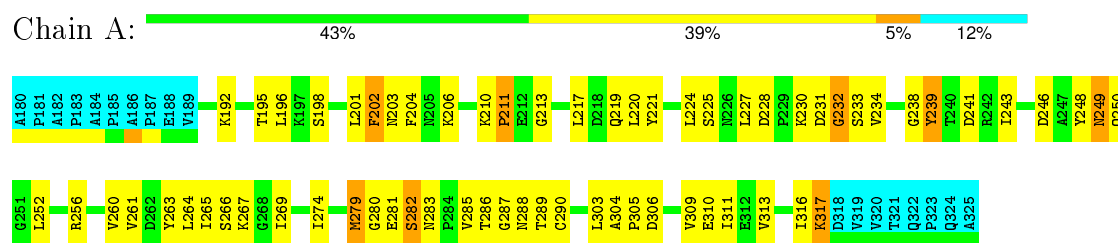
- Molecule 1: OmpA domain protein transmembrane region-containing protein





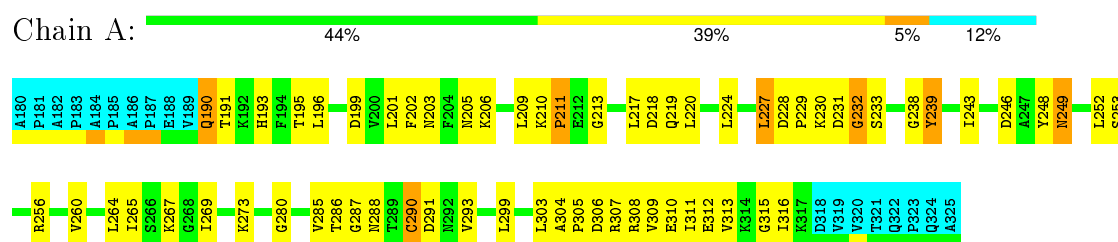
#### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: OmpA domain protein transmembrane region-containing protein



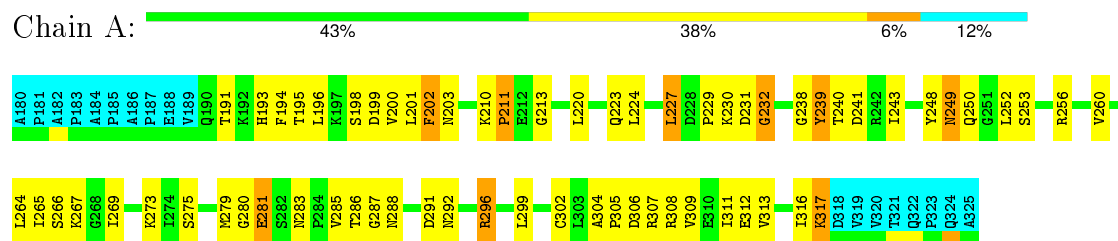
#### 4.2.15 Score per residue for model 15

- Molecule 1: OmpA domain protein transmembrane region-containing protein



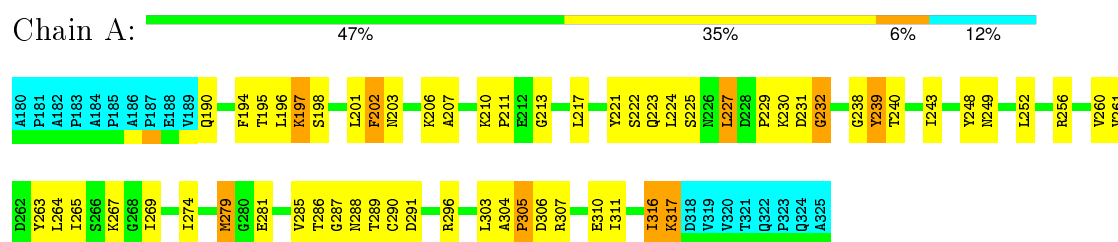
#### 4.2.16 Score per residue for model 16

- Molecule 1: OmpA domain protein transmembrane region-containing protein



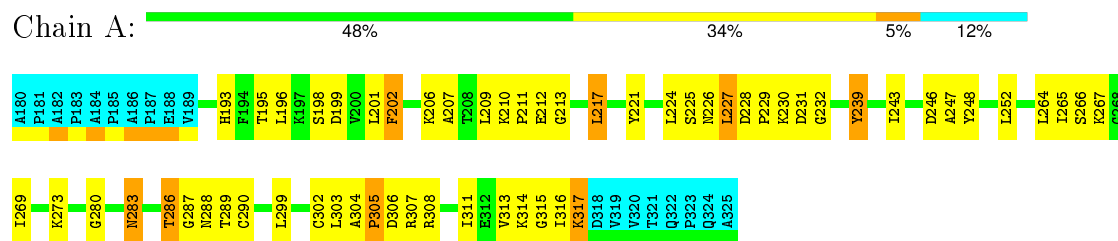
#### 4.2.17 Score per residue for model 17

- Molecule 1: OmpA domain protein transmembrane region-containing protein



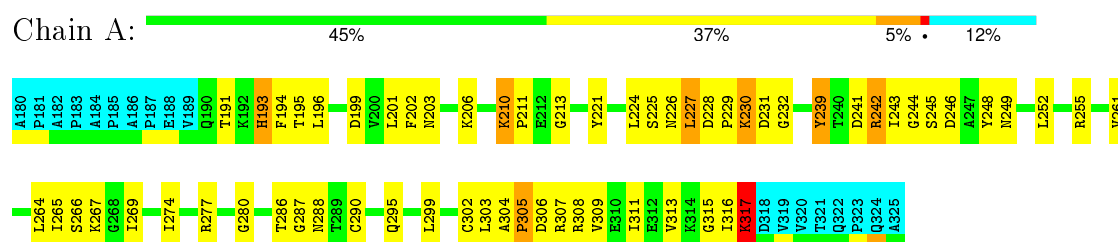
### 4.2.18 Score per residue for model 18

- Molecule 1: OmpA domain protein transmembrane region-containing protein



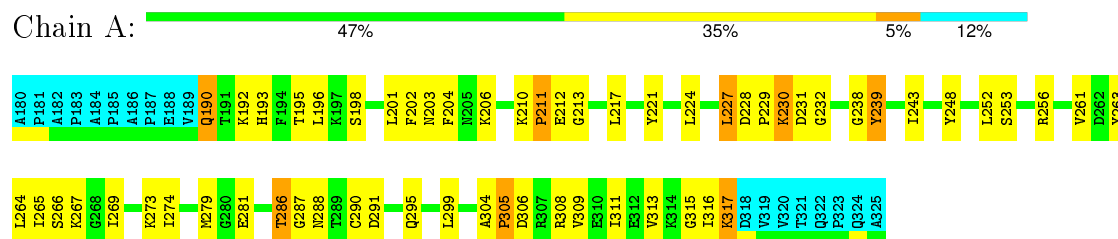
### 4.2.19 Score per residue for model 19

- Molecule 1: OmpA domain protein transmembrane region-containing protein



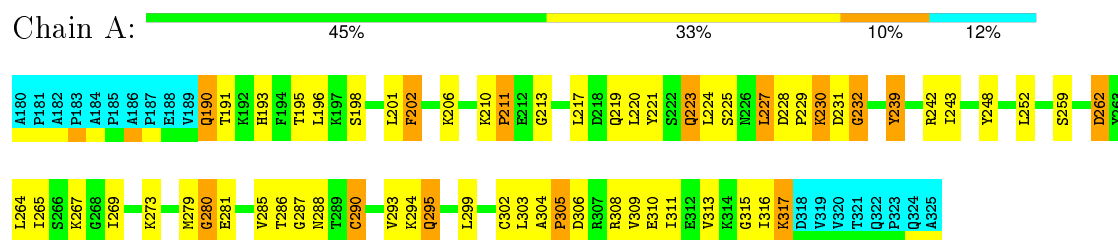
### 4.2.20 Score per residue for model 20

- Molecule 1: OmpA domain protein transmembrane region-containing protein



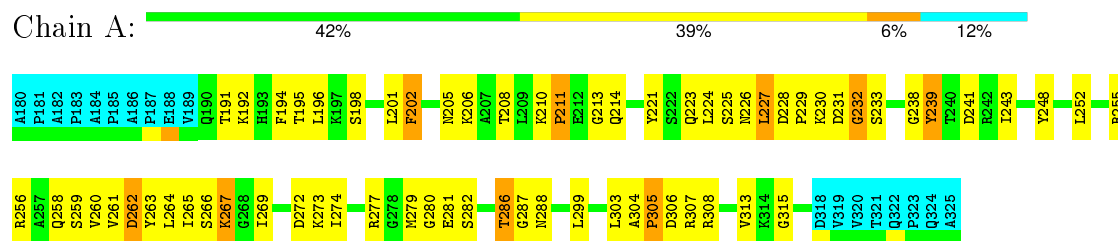
### 4.2.21 Score per residue for model 21

- Molecule 1: OmpA domain protein transmembrane region-containing protein



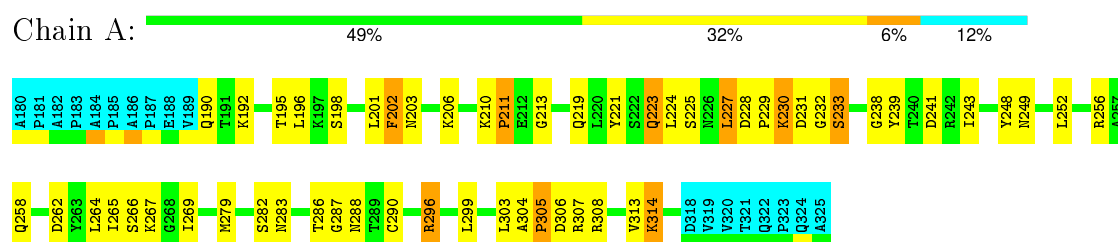
#### 4.2.22 Score per residue for model 22

- Molecule 1: OmpA domain protein transmembrane region-containing protein



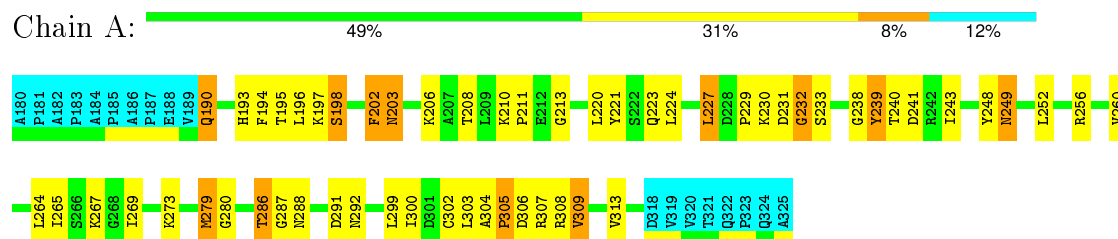
#### 4.2.23 Score per residue for model 23

- Molecule 1: OmpA domain protein transmembrane region-containing protein



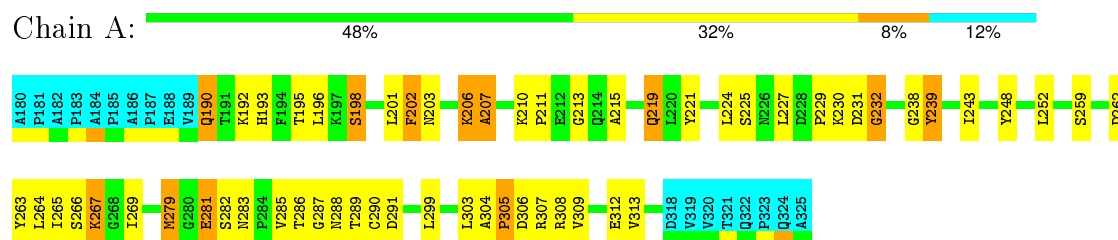
#### 4.2.24 Score per residue for model 24

- Molecule 1: OmpA domain protein transmembrane region-containing protein



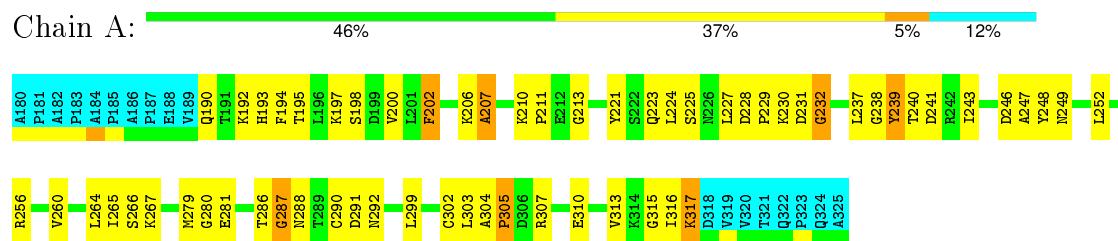
#### 4.2.25 Score per residue for model 25

- Molecule 1: OmpA domain protein transmembrane region-containing protein



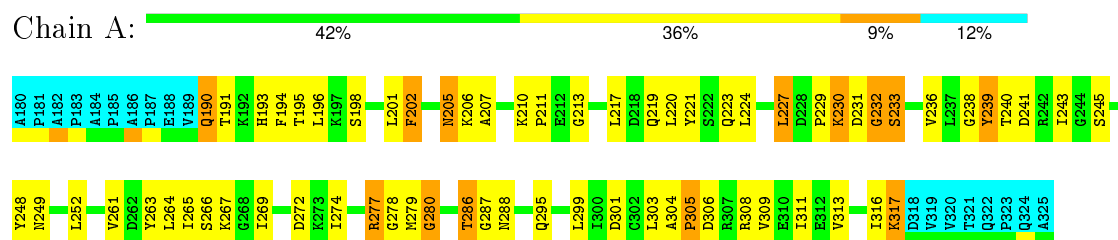
### 4.2.26 Score per residue for model 26

- Molecule 1: OmpA domain protein transmembrane region-containing protein



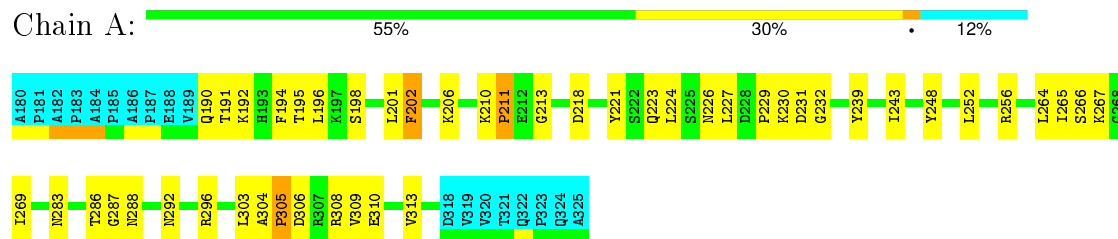
### 4.2.27 Score per residue for model 27

- Molecule 1: OmpA domain protein transmembrane region-containing protein



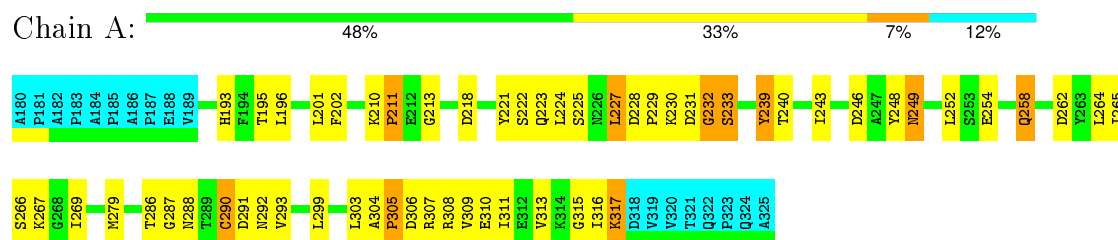
### 4.2.28 Score per residue for model 28

- Molecule 1: OmpA domain protein transmembrane region-containing protein



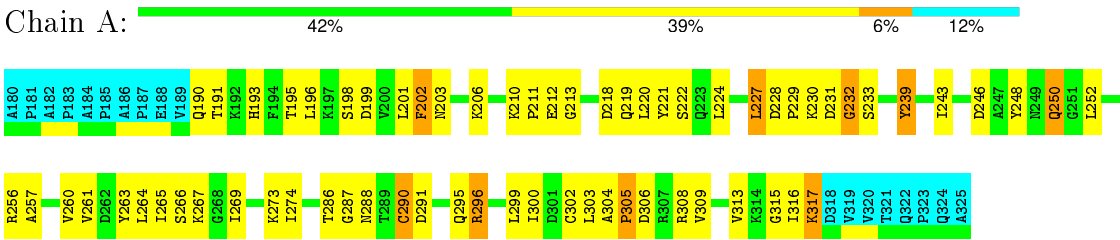
### 4.2.29 Score per residue for model 29

- Molecule 1: OmpA domain protein transmembrane region-containing protein



4.2.30 Score per residue for model 30

- Molecule 1: OmpA domain protein transmembrane region-containing protein



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 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
CYANA	structure solution	2.0
X-PLOR NIH	structure solution	2.20
X-PLOR NIH	refinement	2.20
CYANA	refinement	2.0

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)	2mqe_cs.str
Number of chemical shift lists	1
Total number of shifts	254
Number of shifts mapped to atoms	254
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%

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	979	987	986	51±5
All	All	29370	29610	29580	1521

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:224:LEU:HD22	1:A:313:VAL:HG21	0.87	1.46	7	24
1:A:252:LEU:HD23	1:A:255:ARG:HE	0.86	1.27	4	1
1:A:316:ILE:O	1:A:317:LYS:O	0.83	1.96	14	16
1:A:256:ARG:O	1:A:260:VAL:HG23	0.79	1.78	30	13
1:A:259:SER:O	1:A:262:ASP:OD1	0.78	2.01	25	2
1:A:223:GLN:H	1:A:223:GLN:HE21	0.77	1.20	21	1
1:A:223:GLN:HE21	1:A:223:GLN:H	0.75	1.22	11	2
1:A:248:TYR:CE2	1:A:252:LEU:HD11	0.70	2.21	4	28
1:A:286:THR:HG21	1:A:302:CYS:O	0.69	1.87	21	4
1:A:252:LEU:HD23	1:A:255:ARG:NE	0.69	2.00	4	1
1:A:223:GLN:H	1:A:223:GLN:NE2	0.69	1.86	21	1
1:A:243:ILE:O	1:A:243:ILE:HG22	0.68	1.89	9	20
1:A:196:LEU:HD23	1:A:201:LEU:HD11	0.67	1.64	18	23
1:A:223:GLN:N	1:A:223:GLN:NE2	0.67	2.42	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:243:ILE:HG22	1:A:243:ILE:O	0.67	1.89	16	10
1:A:190:GLN:H	1:A:190:GLN:NE2	0.66	1.89	15	1
1:A:196:LEU:CD2	1:A:201:LEU:HD11	0.66	2.20	15	28
1:A:205:ASN:H	1:A:205:ASN:ND2	0.66	1.89	27	1
1:A:223:GLN:NE2	1:A:223:GLN:N	0.66	2.43	23	2
1:A:262:ASP:OD1	1:A:263:TYR:N	0.66	2.28	25	2
1:A:223:GLN:NE2	1:A:223:GLN:H	0.65	1.89	23	2
1:A:304:ALA:N	1:A:305:PRO:CD	0.65	2.59	5	28
1:A:228:ASP:N	1:A:315:GLY:O	0.65	2.30	18	15
1:A:224:LEU:O	1:A:227:LEU:HD22	0.65	1.91	29	19
1:A:194:PHE:CZ	1:A:223:GLN:NE2	0.65	2.65	1	15
1:A:194:PHE:CE1	1:A:223:GLN:NE2	0.64	2.64	28	8
1:A:256:ARG:HH22	1:A:308:ARG:N	0.64	1.90	23	3
1:A:263:TYR:CE2	1:A:267:LYS:NZ	0.64	2.66	10	5
1:A:263:TYR:CZ	1:A:267:LYS:NZ	0.64	2.66	9	4
1:A:286:THR:O	1:A:288:ASN:N	0.64	2.31	4	28
1:A:239:TYR:CZ	1:A:279:MET:SD	0.64	2.91	29	3
1:A:239:TYR:N	1:A:239:TYR:CD1	0.63	2.65	10	11
1:A:206:LYS:NZ	1:A:255:ARG:NH1	0.63	2.47	13	1
1:A:239:TYR:CE2	1:A:279:MET:SD	0.63	2.92	13	4
1:A:238:GLY:O	1:A:279:MET:N	0.63	2.32	7	12
1:A:194:PHE:CE2	1:A:223:GLN:NE2	0.62	2.67	27	5
1:A:239:TYR:CD1	1:A:239:TYR:N	0.62	2.67	2	15
1:A:287:GLY:O	1:A:290:CYS:N	0.62	2.32	7	2
1:A:286:THR:OG1	1:A:303:LEU:HD23	0.62	1.95	23	3
1:A:199:ASP:OD1	1:A:200:VAL:N	0.61	2.33	16	1
1:A:205:ASN:HD22	1:A:210:LYS:NZ	0.61	1.92	15	1
1:A:204:PHE:CE2	1:A:205:ASN:ND2	0.61	2.69	5	1
1:A:205:ASN:HD22	1:A:205:ASN:H	0.61	1.38	27	1
1:A:290:CYS:SG	1:A:293:VAL:HG21	0.61	2.36	2	9
1:A:242:ARG:NH1	1:A:245:SER:N	0.60	2.49	19	1
1:A:223:GLN:HE21	1:A:223:GLN:N	0.60	1.90	11	1
1:A:256:ARG:NH2	1:A:308:ARG:O	0.60	2.34	28	1
1:A:193:HIS:ND1	1:A:193:HIS:N	0.60	2.49	7	2
1:A:195:THR:O	1:A:195:THR:HG23	0.60	1.97	24	6
1:A:204:PHE:CE1	1:A:205:ASN:ND2	0.60	2.70	2	1
1:A:223:GLN:N	1:A:223:GLN:HE21	0.59	1.91	21	2
1:A:256:ARG:HH22	1:A:307:ARG:HE	0.59	1.39	22	1
1:A:191:THR:HG22	1:A:192:LYS:N	0.59	2.13	28	3
1:A:298:ALA:O	1:A:301:ASP:OD1	0.59	2.19	7	1
1:A:203:ASN:ND2	1:A:204:PHE:CE2	0.59	2.70	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:263:TYR:CE2	1:A:267:LYS:CE	0.59	2.86	17	12
1:A:267:LYS:CD	1:A:267:LYS:N	0.59	2.66	13	1
1:A:203:ASN:HD22	1:A:307:ARG:HH11	0.58	1.42	24	1
1:A:299:LEU:O	1:A:303:LEU:N	0.58	2.37	24	22
1:A:240:THR:HG22	1:A:241:ASP:N	0.58	2.12	10	5
1:A:277:ARG:NH1	1:A:278:GLY:O	0.58	2.36	27	1
1:A:229:PRO:O	1:A:232:GLY:N	0.57	2.36	19	11
1:A:301:ASP:OD1	1:A:302:CYS:N	0.57	2.36	7	1
1:A:242:ARG:NE	1:A:281:GLU:OE1	0.57	2.37	21	1
1:A:195:THR:HG23	1:A:195:THR:O	0.57	1.99	10	1
1:A:298:ALA:C	1:A:301:ASP:OD1	0.57	2.43	7	1
1:A:202:PHE:CD2	1:A:207:ALA:O	0.57	2.58	3	10
1:A:198:SER:OG	1:A:256:ARG:NH2	0.57	2.37	1	4
1:A:227:LEU:O	1:A:227:LEU:HD23	0.57	2.00	30	7
1:A:286:THR:C	1:A:288:ASN:H	0.57	2.03	5	28
1:A:239:TYR:CD1	1:A:308:ARG:O	0.56	2.58	25	19
1:A:227:LEU:HD23	1:A:227:LEU:O	0.56	2.00	29	4
1:A:210:LYS:O	1:A:213:GLY:N	0.56	2.39	21	30
1:A:248:TYR:CZ	1:A:252:LEU:HD11	0.56	2.35	28	30
1:A:256:ARG:NH2	1:A:308:ARG:N	0.56	2.53	23	1
1:A:263:TYR:CE1	1:A:267:LYS:NZ	0.56	2.67	3	2
1:A:228:ASP:OD1	1:A:230:LYS:N	0.56	2.39	23	1
1:A:239:TYR:O	1:A:256:ARG:NH2	0.56	2.40	28	1
1:A:256:ARG:NH2	1:A:307:ARG:HE	0.55	1.99	22	1
1:A:261:VAL:HG21	1:A:276:ALA:HB2	0.55	1.79	2	3
1:A:296:ARG:O	1:A:299:LEU:N	0.55	2.40	23	3
1:A:258:GLN:NE2	1:A:262:ASP:OD2	0.55	2.40	29	1
1:A:279:MET:O	1:A:280:GLY:C	0.55	2.45	7	5
1:A:252:LEU:CD2	1:A:255:ARG:HH21	0.55	2.14	4	1
1:A:246:ASP:O	1:A:250:GLN:NE2	0.55	2.40	30	1
1:A:277:ARG:NH1	1:A:279:MET:SD	0.55	2.80	9	1
1:A:203:ASN:ND2	1:A:307:ARG:HH11	0.55	2.00	24	1
1:A:252:LEU:HD22	1:A:256:ARG:HH12	0.54	1.61	7	1
1:A:240:THR:OG1	1:A:249:ASN:ND2	0.54	2.40	4	1
1:A:219:GLN:O	1:A:223:GLN:NE2	0.54	2.40	23	3
1:A:316:ILE:CG1	1:A:317:LYS:N	0.54	2.70	11	17
1:A:212:GLU:CD	1:A:212:GLU:H	0.54	2.06	20	3
1:A:304:ALA:O	1:A:306:ASP:N	0.54	2.40	18	7
1:A:308:ARG:NH1	1:A:310:GLU:OE2	0.54	2.40	29	2
1:A:198:SER:O	1:A:202:PHE:N	0.54	2.40	26	15
1:A:241:ASP:OD2	1:A:307:ARG:NH2	0.54	2.40	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:ASN:O	1:A:307:ARG:NH2	0.54	2.41	17	3
1:A:203:ASN:O	1:A:307:ARG:NH1	0.54	2.41	23	2
1:A:201:LEU:HD22	1:A:209:LEU:HD22	0.54	1.80	18	2
1:A:304:ALA:N	1:A:305:PRO:HD2	0.54	2.18	6	3
1:A:256:ARG:NH2	1:A:307:ARG:HH21	0.54	1.99	6	2
1:A:190:GLN:NE2	1:A:316:ILE:O	0.54	2.40	15	1
1:A:218:ASP:OD1	1:A:267:LYS:NZ	0.54	2.39	28	5
1:A:206:LYS:C	1:A:255:ARG:HH22	0.54	2.06	4	1
1:A:242:ARG:NH2	1:A:246:ASP:OD1	0.54	2.41	19	1
1:A:241:ASP:O	1:A:249:ASN:ND2	0.54	2.39	4	5
1:A:281:GLU:OE1	1:A:281:GLU:N	0.53	2.41	7	1
1:A:312:GLU:OE1	1:A:312:GLU:N	0.53	2.41	9	1
1:A:291:ASP:OD1	1:A:292:ASN:N	0.53	2.42	16	2
1:A:239:TYR:N	1:A:256:ARG:HH22	0.53	2.01	15	1
1:A:286:THR:C	1:A:288:ASN:N	0.53	2.60	4	28
1:A:267:LYS:N	1:A:267:LYS:CD	0.53	2.72	9	1
1:A:205:ASN:ND2	1:A:208:THR:OG1	0.53	2.41	11	3
1:A:199:ASP:OD1	1:A:307:ARG:NE	0.53	2.42	18	1
1:A:205:ASN:ND2	1:A:210:LYS:HZ1	0.53	2.02	15	1
1:A:205:ASN:ND2	1:A:210:LYS:NZ	0.53	2.56	15	1
1:A:246:ASP:O	1:A:249:ASN:ND2	0.53	2.42	15	1
1:A:265:ILE:O	1:A:267:LYS:N	0.53	2.42	13	26
1:A:250:GLN:N	1:A:250:GLN:OE1	0.53	2.42	30	1
1:A:199:ASP:OD2	1:A:307:ARG:NH2	0.53	2.42	18	1
1:A:193:HIS:N	1:A:193:HIS:CD2	0.53	2.76	10	4
1:A:249:ASN:ND2	1:A:281:GLU:OE2	0.53	2.41	26	1
1:A:283:ASN:O	1:A:283:ASN:ND2	0.53	2.42	18	1
1:A:241:ASP:OD2	1:A:307:ARG:NE	0.53	2.42	11	2
1:A:229:PRO:O	1:A:231:ASP:N	0.53	2.42	19	5
1:A:193:HIS:CD2	1:A:193:HIS:N	0.52	2.76	15	2
1:A:242:ARG:NE	1:A:244:GLY:H	0.52	2.02	2	1
1:A:221:TYR:CZ	1:A:267:LYS:O	0.52	2.63	13	15
1:A:299:LEU:O	1:A:302:CYS:N	0.52	2.42	24	1
1:A:203:ASN:ND2	1:A:210:LYS:NZ	0.52	2.57	6	1
1:A:231:ASP:O	1:A:233:SER:N	0.52	2.42	27	9
1:A:224:LEU:HD22	1:A:313:VAL:CG2	0.52	2.33	1	3
1:A:193:HIS:N	1:A:193:HIS:ND1	0.52	2.57	19	1
1:A:272:ASP:OD1	1:A:273:LYS:N	0.52	2.43	2	3
1:A:281:GLU:N	1:A:281:GLU:OE1	0.52	2.42	20	1
1:A:221:TYR:O	1:A:225:SER:N	0.52	2.43	6	13
1:A:206:LYS:CG	1:A:207:ALA:H	0.52	2.18	26	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:241:ASP:OD1	1:A:241:ASP:N	0.52	2.43	14	2
1:A:286:THR:O	1:A:290:CYS:N	0.51	2.39	26	8
1:A:304:ALA:C	1:A:306:ASP:H	0.51	2.09	18	22
1:A:290:CYS:SG	1:A:302:CYS:O	0.51	2.68	1	2
1:A:239:TYR:O	1:A:256:ARG:NH1	0.51	2.43	8	5
1:A:316:ILE:CG1	1:A:317:LYS:H	0.51	2.18	11	5
1:A:306:ASP:N	1:A:306:ASP:OD1	0.51	2.43	9	1
1:A:265:ILE:C	1:A:267:LYS:H	0.51	2.10	13	26
1:A:287:GLY:O	1:A:288:ASN:C	0.51	2.49	7	2
1:A:265:ILE:C	1:A:267:LYS:N	0.51	2.64	23	30
1:A:233:SER:N	1:A:314:LYS:HZ2	0.51	2.04	23	1
1:A:314:LYS:O	1:A:315:GLY:C	0.51	2.49	12	1
1:A:198:SER:OG	1:A:256:ARG:NH1	0.51	2.44	2	1
1:A:279:MET:CE	1:A:282:SER:H	0.51	2.19	22	2
1:A:207:ALA:HB2	1:A:255:ARG:NH1	0.51	2.21	4	1
1:A:229:PRO:O	1:A:230:LYS:C	0.50	2.50	20	28
1:A:233:SER:H	1:A:314:LYS:HD2	0.50	1.66	12	2
1:A:192:LYS:O	1:A:193:HIS:CG	0.50	2.65	20	4
1:A:201:LEU:O	1:A:210:LYS:CG	0.50	2.60	19	1
1:A:198:SER:OG	1:A:202:PHE:O	0.50	2.29	6	2
1:A:192:LYS:C	1:A:193:HIS:CG	0.50	2.84	9	6
1:A:295:GLN:HE22	1:A:296:ARG:CZ	0.50	2.20	30	1
1:A:194:PHE:CE2	1:A:224:LEU:HD21	0.50	2.42	22	2
1:A:190:GLN:N	1:A:190:GLN:CD	0.50	2.65	17	3
1:A:192:LYS:O	1:A:193:HIS:CD2	0.50	2.65	8	2
1:A:191:THR:HG22	1:A:193:HIS:CE1	0.50	2.41	19	4
1:A:206:LYS:CG	1:A:207:ALA:N	0.50	2.75	9	2
1:A:239:TYR:CZ	1:A:310:GLU:CD	0.50	2.85	28	3
1:A:238:GLY:HA2	1:A:309:VAL:HG12	0.50	1.83	11	5
1:A:243:ILE:CG2	1:A:243:ILE:O	0.49	2.60	28	17
1:A:296:ARG:O	1:A:300:ILE:N	0.49	2.43	30	1
1:A:240:THR:CG2	1:A:241:ASP:N	0.49	2.75	10	4
1:A:240:THR:OG1	1:A:256:ARG:NH1	0.49	2.45	3	1
1:A:239:TYR:CD2	1:A:279:MET:SD	0.49	3.06	22	1
1:A:203:ASN:OD1	1:A:204:PHE:CD2	0.49	2.64	10	1
1:A:285:VAL:HG23	1:A:286:THR:N	0.49	2.22	14	11
1:A:249:ASN:ND2	1:A:250:GLN:N	0.49	2.60	16	2
1:A:283:ASN:N	1:A:283:ASN:ND2	0.49	2.58	8	1
1:A:203:ASN:OD1	1:A:204:PHE:CE2	0.49	2.66	10	1
1:A:243:ILE:O	1:A:243:ILE:CG2	0.49	2.61	24	12
1:A:199:ASP:OD1	1:A:307:ARG:NH1	0.49	2.46	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:ASN:ND2	1:A:307:ARG:NH1	0.49	2.60	24	1
1:A:314:LYS:O	1:A:314:LYS:NZ	0.49	2.45	12	1
1:A:203:ASN:O	1:A:307:ARG:CZ	0.49	2.61	6	1
1:A:197:LYS:O	1:A:200:VAL:HG22	0.49	2.08	26	1
1:A:261:VAL:HG13	1:A:274:ILE:HD12	0.49	1.83	17	13
1:A:194:PHE:CE1	1:A:224:LEU:HD21	0.49	2.42	27	3
1:A:199:ASP:OD1	1:A:307:ARG:NH2	0.49	2.46	9	1
1:A:279:MET:O	1:A:281:GLU:N	0.49	2.44	10	5
1:A:198:SER:O	1:A:202:PHE:O	0.49	2.30	16	15
1:A:239:TYR:CZ	1:A:310:GLU:OE1	0.49	2.66	28	1
1:A:240:THR:HG23	1:A:249:ASN:ND2	0.49	2.23	17	1
1:A:239:TYR:C	1:A:256:ARG:NH2	0.49	2.66	15	1
1:A:245:SER:O	1:A:249:ASN:OD1	0.48	2.31	27	1
1:A:195:THR:OG1	1:A:308:ARG:NH2	0.48	2.46	6	2
1:A:281:GLU:CD	1:A:281:GLU:N	0.48	2.67	6	2
1:A:231:ASP:O	1:A:232:GLY:C	0.48	2.52	27	30
1:A:237:LEU:HD22	1:A:279:MET:SD	0.48	2.48	26	1
1:A:279:MET:SD	1:A:282:SER:OG	0.48	2.70	7	1
1:A:242:ARG:CZ	1:A:281:GLU:OE1	0.48	2.61	10	1
1:A:190:GLN:CD	1:A:190:GLN:N	0.48	2.66	1	8
1:A:314:LYS:HG2	1:A:315:GLY:N	0.48	2.24	12	1
1:A:238:GLY:O	1:A:253:SER:OG	0.48	2.32	20	3
1:A:258:GLN:HE21	1:A:258:GLN:C	0.48	2.12	29	1
1:A:258:GLN:NE2	1:A:262:ASP:CG	0.48	2.67	29	1
1:A:256:ARG:CG	1:A:257:ALA:N	0.48	2.77	1	1
1:A:279:MET:HE2	1:A:282:SER:H	0.48	1.69	22	1
1:A:238:GLY:O	1:A:279:MET:CB	0.48	2.62	11	5
1:A:221:TYR:O	1:A:225:SER:OG	0.48	2.32	1	4
1:A:259:SER:O	1:A:262:ASP:OD2	0.48	2.32	22	2
1:A:233:SER:H	1:A:314:LYS:CE	0.47	2.22	23	2
1:A:314:LYS:HZ3	1:A:315:GLY:CA	0.47	2.22	12	1
1:A:230:LYS:CG	1:A:231:ASP:N	0.47	2.77	6	1
1:A:253:SER:OG	1:A:278:GLY:CA	0.47	2.62	5	1
1:A:249:ASN:C	1:A:249:ASN:ND2	0.47	2.67	16	2
1:A:228:ASP:CB	1:A:315:GLY:O	0.47	2.62	15	3
1:A:239:TYR:CG	1:A:279:MET:SD	0.47	3.07	22	1
1:A:295:GLN:O	1:A:299:LEU:HD12	0.47	2.10	13	4
1:A:243:ILE:H	1:A:249:ASN:HD21	0.47	1.53	23	1
1:A:279:MET:C	1:A:279:MET:SD	0.47	2.92	22	1
1:A:239:TYR:OH	1:A:310:GLU:OE1	0.47	2.33	12	4
1:A:304:ALA:C	1:A:307:ARG:NH1	0.47	2.68	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:233:SER:H	1:A:314:LYS:NZ	0.47	2.08	23	1
1:A:234:VAL:HG22	1:A:313:VAL:HG22	0.47	1.86	14	2
1:A:314:LYS:NZ	1:A:315:GLY:O	0.47	2.47	12	1
1:A:283:ASN:C	1:A:283:ASN:HD22	0.47	2.13	18	1
1:A:251:GLY:C	1:A:255:ARG:NH2	0.47	2.67	7	1
1:A:203:ASN:OD1	1:A:307:ARG:NH1	0.47	2.47	7	2
1:A:285:VAL:CG2	1:A:286:THR:N	0.47	2.78	14	5
1:A:218:ASP:CG	1:A:267:LYS:NZ	0.47	2.68	30	2
1:A:314:LYS:H	1:A:314:LYS:HD3	0.47	1.70	23	1
1:A:206:LYS:NZ	1:A:255:ARG:HH11	0.47	2.08	13	1
1:A:203:ASN:N	1:A:203:ASN:OD1	0.47	2.45	16	4
1:A:258:GLN:NE2	1:A:258:GLN:C	0.47	2.68	29	1
1:A:215:ALA:O	1:A:219:GLN:NE2	0.47	2.48	25	1
1:A:307:ARG:O	1:A:307:ARG:CG	0.46	2.63	17	4
1:A:192:LYS:N	1:A:313:VAL:O	0.46	2.45	14	5
1:A:223:GLN:OE1	1:A:316:ILE:HD11	0.46	2.10	29	1
1:A:203:ASN:HD22	1:A:210:LYS:NZ	0.46	2.09	2	2
1:A:258:GLN:O	1:A:262:ASP:OD1	0.46	2.33	6	1
1:A:237:LEU:HD21	1:A:277:ARG:NE	0.46	2.25	10	1
1:A:222:SER:O	1:A:225:SER:N	0.46	2.48	29	3
1:A:199:ASP:O	1:A:203:ASN:ND2	0.46	2.47	12	3
1:A:246:ASP:N	1:A:246:ASP:OD1	0.46	2.46	2	2
1:A:219:GLN:CG	1:A:220:LEU:N	0.46	2.79	14	5
1:A:279:MET:HE3	1:A:282:SER:H	0.46	1.69	14	1
1:A:241:ASP:OD2	1:A:243:ILE:HD11	0.46	2.11	22	1
1:A:196:LEU:HD21	1:A:201:LEU:HD11	0.46	1.88	4	4
1:A:304:ALA:HB3	1:A:305:PRO:HD3	0.46	1.87	23	8
1:A:191:THR:HG22	1:A:193:HIS:NE2	0.46	2.25	15	3
1:A:303:LEU:O	1:A:306:ASP:OD1	0.46	2.33	10	2
1:A:287:GLY:O	1:A:291:ASP:N	0.46	2.49	26	1
1:A:228:ASP:OD1	1:A:230:LYS:CB	0.46	2.64	23	1
1:A:210:LYS:NZ	1:A:210:LYS:CB	0.46	2.79	27	1
1:A:231:ASP:O	1:A:233:SER:OG	0.46	2.31	29	1
1:A:199:ASP:OD1	1:A:203:ASN:ND2	0.46	2.49	30	1
1:A:240:THR:CG2	1:A:249:ASN:ND2	0.46	2.78	17	1
1:A:227:LEU:CD2	1:A:227:LEU:H	0.45	2.24	22	1
1:A:304:ALA:HB1	1:A:307:ARG:NH1	0.45	2.26	25	1
1:A:239:TYR:HB2	1:A:308:ARG:O	0.45	2.11	23	4
1:A:306:ASP:OD1	1:A:306:ASP:O	0.45	2.34	22	10
1:A:221:TYR:C	1:A:223:GLN:N	0.45	2.69	27	3
1:A:191:THR:CG2	1:A:192:LYS:N	0.45	2.80	28	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:269:ILE:CG2	1:A:269:ILE:O	0.45	2.63	9	1
1:A:220:LEU:O	1:A:224:LEU:HG	0.45	2.12	24	4
1:A:190:GLN:N	1:A:190:GLN:NE2	0.45	2.62	15	2
1:A:190:GLN:CD	1:A:190:GLN:H	0.45	2.15	15	1
1:A:236:VAL:HG21	1:A:261:VAL:CG2	0.45	2.42	27	3
1:A:221:TYR:CE1	1:A:225:SER:OG	0.45	2.61	26	2
1:A:279:MET:CE	1:A:282:SER:OG	0.45	2.65	22	1
1:A:239:TYR:CZ	1:A:310:GLU:OE2	0.45	2.70	21	2
1:A:246:ASP:OD1	1:A:247:ALA:N	0.45	2.50	18	1
1:A:203:ASN:CG	1:A:204:PHE:H	0.45	2.15	20	1
1:A:285:VAL:HG23	1:A:286:THR:H	0.45	1.72	21	1
1:A:246:ASP:CG	1:A:247:ALA:N	0.45	2.70	26	2
1:A:291:ASP:OD1	1:A:291:ASP:N	0.45	2.50	9	6
1:A:306:ASP:O	1:A:306:ASP:OD1	0.45	2.35	24	6
1:A:215:ALA:O	1:A:219:GLN:CD	0.44	2.56	25	1
1:A:219:GLN:O	1:A:222:SER:OG	0.44	2.35	30	1
1:A:272:ASP:O	1:A:272:ASP:OD1	0.44	2.35	27	3
1:A:239:TYR:HD1	1:A:239:TYR:N	0.44	2.10	9	5
1:A:281:GLU:OE1	1:A:306:ASP:OD1	0.44	2.36	14	1
1:A:226:ASN:OD1	1:A:226:ASN:O	0.44	2.35	22	2
1:A:312:GLU:OE1	1:A:312:GLU:O	0.44	2.35	15	1
1:A:221:TYR:CD1	1:A:267:LYS:CB	0.44	3.01	27	15
1:A:193:HIS:CE1	1:A:312:GLU:OE2	0.44	2.70	25	1
1:A:227:LEU:CD2	1:A:227:LEU:N	0.44	2.80	22	2
1:A:281:GLU:OE2	1:A:306:ASP:OD2	0.44	2.36	17	2
1:A:239:TYR:CE2	1:A:279:MET:CE	0.44	3.01	29	2
1:A:240:THR:O	1:A:306:ASP:OD1	0.44	2.36	29	1
1:A:198:SER:OG	1:A:307:ARG:C	0.44	2.56	1	1
1:A:223:GLN:O	1:A:226:ASN:OD1	0.44	2.35	28	1
1:A:211:PRO:C	1:A:213:GLY:N	0.44	2.71	28	8
1:A:256:ARG:O	1:A:260:VAL:CG2	0.44	2.61	8	1
1:A:224:LEU:CD2	1:A:313:VAL:HG21	0.44	2.41	30	5
1:A:210:LYS:O	1:A:211:PRO:C	0.44	2.56	21	11
1:A:233:SER:H	1:A:314:LYS:CD	0.44	2.26	12	2
1:A:264:LEU:O	1:A:264:LEU:HD23	0.44	2.12	3	1
1:A:312:GLU:CA	1:A:312:GLU:OE1	0.44	2.66	9	1
1:A:249:ASN:O	1:A:253:SER:OG	0.44	2.34	11	1
1:A:283:ASN:N	1:A:283:ASN:OD1	0.44	2.51	25	2
1:A:291:ASP:OD1	1:A:291:ASP:O	0.44	2.36	12	4
1:A:256:ARG:HG3	1:A:257:ALA:N	0.44	2.28	8	2
1:A:303:LEU:O	1:A:306:ASP:CG	0.44	2.56	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:233:SER:H	1:A:314:LYS:HZ2	0.44	1.56	23	1
1:A:262:ASP:N	1:A:262:ASP:OD1	0.44	2.48	6	1
1:A:191:THR:HG22	1:A:192:LYS:H	0.43	1.73	28	2
1:A:241:ASP:O	1:A:249:ASN:OD1	0.43	2.36	23	2
1:A:288:ASN:O	1:A:291:ASP:OD2	0.43	2.36	20	1
1:A:228:ASP:OD2	1:A:230:LYS:CG	0.43	2.66	14	1
1:A:192:LYS:C	1:A:193:HIS:CD2	0.43	2.91	25	1
1:A:190:GLN:NE2	1:A:190:GLN:H	0.43	2.12	28	2
1:A:201:LEU:HD21	1:A:217:LEU:HD23	0.43	1.89	18	1
1:A:295:GLN:O	1:A:299:LEU:CD1	0.43	2.66	13	2
1:A:260:VAL:O	1:A:264:LEU:N	0.43	2.47	6	1
1:A:283:ASN:ND2	1:A:308:ARG:NH2	0.43	2.66	18	1
1:A:239:TYR:N	1:A:239:TYR:HD1	0.43	2.12	27	6
1:A:226:ASN:O	1:A:226:ASN:OD1	0.43	2.36	12	2
1:A:292:ASN:OD1	1:A:292:ASN:O	0.43	2.36	26	1
1:A:281:GLU:O	1:A:281:GLU:OE1	0.43	2.37	13	2
1:A:199:ASP:OD1	1:A:203:ASN:OD1	0.43	2.37	11	2
1:A:316:ILE:HG12	1:A:317:LYS:N	0.43	2.28	11	1
1:A:291:ASP:O	1:A:291:ASP:OD1	0.43	2.37	15	1
1:A:238:GLY:O	1:A:279:MET:SD	0.43	2.77	22	1
1:A:198:SER:CB	1:A:202:PHE:O	0.43	2.67	26	1
1:A:237:LEU:HD23	1:A:277:ARG:HB3	0.43	1.91	5	1
1:A:205:ASN:N	1:A:205:ASN:ND2	0.43	2.64	27	1
1:A:202:PHE:CD1	1:A:256:ARG:NH1	0.43	2.87	9	1
1:A:249:ASN:HD21	1:A:280:GLY:CA	0.43	2.27	24	1
1:A:246:ASP:O	1:A:249:ASN:OD1	0.43	2.37	29	2
1:A:237:LEU:CD2	1:A:277:ARG:HE	0.43	2.27	10	1
1:A:220:LEU:HD12	1:A:223:GLN:HE21	0.43	1.74	7	1
1:A:263:TYR:O	1:A:267:LYS:CE	0.43	2.67	9	1
1:A:281:GLU:OE1	1:A:281:GLU:O	0.43	2.37	25	1
1:A:245:SER:O	1:A:248:TYR:N	0.42	2.52	27	1
1:A:263:TYR:O	1:A:267:LYS:NZ	0.42	2.52	9	1
1:A:206:LYS:HG3	1:A:207:ALA:N	0.42	2.29	9	1
1:A:240:THR:CG2	1:A:249:ASN:CG	0.42	2.87	17	1
1:A:242:ARG:NH1	1:A:244:GLY:C	0.42	2.72	19	1
1:A:197:LYS:NZ	1:A:199:ASP:OD2	0.42	2.52	6	1
1:A:191:THR:CG2	1:A:193:HIS:NE2	0.42	2.82	16	1
1:A:203:ASN:OD1	1:A:307:ARG:CZ	0.42	2.67	17	1
1:A:221:TYR:CE2	1:A:225:SER:OG	0.42	2.70	13	1
1:A:295:GLN:N	1:A:295:GLN:CD	0.42	2.72	21	1
1:A:240:THR:OG1	1:A:249:ASN:OD1	0.42	2.37	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:THR:CG2	1:A:193:HIS:CE1	0.42	3.03	27	2
1:A:198:SER:OG	1:A:307:ARG:O	0.42	2.34	23	4
1:A:256:ARG:HH22	1:A:308:ARG:H	0.42	1.55	28	1
1:A:206:LYS:C	1:A:255:ARG:HH12	0.42	2.18	4	1
1:A:297:ALA:O	1:A:301:ASP:CG	0.42	2.57	7	1
1:A:195:THR:O	1:A:195:THR:CG2	0.42	2.67	22	3
1:A:239:TYR:CD2	1:A:279:MET:CE	0.42	3.03	14	1
1:A:227:LEU:HD23	1:A:227:LEU:N	0.42	2.30	22	1
1:A:302:CYS:SG	1:A:302:CYS:O	0.42	2.77	24	1
1:A:206:LYS:CA	1:A:255:ARG:HH22	0.42	2.28	4	1
1:A:302:CYS:O	1:A:305:PRO:HD2	0.42	2.14	26	1
1:A:197:LYS:H	1:A:197:LYS:CD	0.42	2.26	17	1
1:A:295:GLN:O	1:A:299:LEU:HD13	0.42	2.15	5	1
1:A:248:TYR:CE2	1:A:252:LEU:CD1	0.42	3.02	7	4
1:A:199:ASP:O	1:A:203:ASN:OD1	0.42	2.37	15	2
1:A:292:ASN:O	1:A:292:ASN:OD1	0.42	2.38	29	1
1:A:249:ASN:OD1	1:A:281:GLU:OE2	0.42	2.37	26	1
1:A:317:LYS:O	1:A:317:LYS:CG	0.42	2.67	12	1
1:A:240:THR:O	1:A:306:ASP:OD2	0.42	2.38	11	1
1:A:203:ASN:HD21	1:A:210:LYS:HZ3	0.42	1.58	6	1
1:A:314:LYS:N	1:A:314:LYS:HD3	0.41	2.29	23	1
1:A:206:LYS:N	1:A:206:LYS:CD	0.41	2.83	15	1
1:A:304:ALA:C	1:A:306:ASP:N	0.41	2.73	18	3
1:A:221:TYR:C	1:A:223:GLN:H	0.41	2.18	27	1
1:A:267:LYS:N	1:A:267:LYS:HD3	0.41	2.31	13	1
1:A:290:CYS:SG	1:A:293:VAL:CG2	0.41	3.08	2	1
1:A:289:THR:CG2	1:A:289:THR:O	0.41	2.68	18	1
1:A:306:ASP:OD1	1:A:306:ASP:N	0.41	2.53	21	1
1:A:241:ASP:CG	1:A:303:LEU:O	0.41	2.59	26	1
1:A:242:ARG:NE	1:A:244:GLY:N	0.41	2.68	2	1
1:A:304:ALA:C	1:A:307:ARG:HH11	0.41	2.18	18	1
1:A:264:LEU:HD23	1:A:264:LEU:O	0.41	2.15	7	1
1:A:202:PHE:CE2	1:A:207:ALA:O	0.41	2.73	3	1
1:A:230:LYS:HG3	1:A:231:ASP:N	0.41	2.31	19	1
1:A:240:THR:OG1	1:A:256:ARG:NH2	0.41	2.53	24	1
1:A:206:LYS:HZ3	1:A:255:ARG:NH1	0.41	2.12	13	1
1:A:242:ARG:NH2	1:A:281:GLU:OE2	0.41	2.53	3	1
1:A:206:LYS:H	1:A:206:LYS:CD	0.41	2.28	15	1
1:A:242:ARG:NH2	1:A:281:GLU:CD	0.41	2.74	10	1
1:A:258:GLN:NE2	1:A:262:ASP:OD1	0.41	2.52	23	1
1:A:282:SER:C	1:A:283:ASN:ND2	0.41	2.74	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:THR:CG2	1:A:195:THR:O	0.41	2.69	28	1
1:A:227:LEU:N	1:A:227:LEU:HD23	0.41	2.31	23	1
1:A:240:THR:CB	1:A:249:ASN:ND2	0.41	2.84	4	1
1:A:198:SER:OG	1:A:307:ARG:CB	0.41	2.68	22	1
1:A:239:TYR:OH	1:A:310:GLU:CD	0.41	2.60	26	1
1:A:304:ALA:O	1:A:307:ARG:CG	0.41	2.69	15	1
1:A:221:TYR:OH	1:A:267:LYS:O	0.41	2.36	8	1
1:A:286:THR:HG21	1:A:303:LEU:HA	0.41	1.93	2	1
1:A:249:ASN:N	1:A:249:ASN:OD1	0.41	2.51	27	1
1:A:299:LEU:O	1:A:300:ILE:C	0.40	2.60	24	1
1:A:241:ASP:O	1:A:281:GLU:OE2	0.40	2.40	7	1
1:A:232:GLY:CA	1:A:314:LYS:HZ2	0.40	2.28	23	1
1:A:240:THR:HG23	1:A:249:ASN:OD1	0.40	2.16	9	1
1:A:196:LEU:HB3	1:A:309:VAL:HG23	0.40	1.92	24	1
1:A:254:GLU:O	1:A:258:GLN:CB	0.40	2.70	29	1
1:A:190:GLN:OE1	1:A:317:LYS:C	0.40	2.60	21	1
1:A:221:TYR:CZ	1:A:225:SER:OG	0.40	2.70	1	1
1:A:214:GLN:NE2	1:A:263:TYR:CE1	0.40	2.89	22	1
1:A:286:THR:HG23	1:A:306:ASP:OD1	0.40	2.17	30	1
1:A:261:VAL:HG13	1:A:274:ILE:CD1	0.40	2.46	27	1
1:A:272:ASP:OD1	1:A:272:ASP:N	0.40	2.52	9	1
1:A:255:ARG:CG	1:A:256:ARG:N	0.40	2.84	4	1
1:A:295:GLN:CA	1:A:295:GLN:OE1	0.40	2.69	1	1
1:A:259:SER:C	1:A:262:ASP:OD1	0.40	2.60	6	1
1:A:240:THR:N	1:A:280:GLY:O	0.40	2.52	27	1
1:A:192:LYS:C	1:A:193:HIS:ND1	0.40	2.74	3	1
1:A:281:GLU:OE2	1:A:306:ASP:CG	0.40	2.60	14	1
1:A:233:SER:H	1:A:314:LYS:HE3	0.40	1.77	12	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	128/146 (88%)	106±2 (83±2%)	15±2 (11±2%)	7±1 (5±1%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3840/4380 (88%)	3193 (83%)	441 (11%)	206 (5%)	4 24

All 13 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	211	PRO	30
1	A	287	GLY	30
1	A	266	SER	23
1	A	232	GLY	23
1	A	305	PRO	22
1	A	280	GLY	19
1	A	206	LYS	19
1	A	317	LYS	17
1	A	230	LYS	9
1	A	207	ALA	6
1	A	296	ARG	5
1	A	316	ILE	2
1	A	315	GLY	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	108/121 (89%)	96±2 (89±2%)	12±2 (11±2%)	12 55
All	All	3240/3630 (89%)	2875 (89%)	365 (11%)	12 55

All 55 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	264	LEU	30
1	A	202	PHE	30
1	A	227	LEU	29
1	A	269	ILE	28
1	A	239	TYR	26
1	A	195	THR	23

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Mol	Chain	Res	Type	Models (Total)
1	A	309	VAL	18
1	A	290	CYS	16
1	A	311	ILE	15
1	A	273	LYS	11
1	A	190	GLN	9
1	A	286	THR	8
1	A	217	LEU	8
1	A	233	SER	7
1	A	283	ASN	7
1	A	258	GLN	7
1	A	289	THR	7
1	A	249	ASN	6
1	A	281	GLU	5
1	A	197	LYS	5
1	A	279	MET	5
1	A	267	LYS	5
1	A	302	CYS	4
1	A	295	GLN	3
1	A	277	ARG	3
1	A	255	ARG	3
1	A	193	HIS	3
1	A	317	LYS	3
1	A	208	THR	3
1	A	223	GLN	3
1	A	312	GLU	3
1	A	303	LEU	3
1	A	242	ARG	2
1	A	282	SER	2
1	A	262	ASP	2
1	A	198	SER	2
1	A	314	LYS	2
1	A	296	ARG	2
1	A	308	ARG	1
1	A	203	ASN	1
1	A	250	GLN	1
1	A	240	THR	1
1	A	228	ASP	1
1	A	219	GLN	1
1	A	306	ASP	1
1	A	192	LYS	1
1	A	256	ARG	1
1	A	205	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	275	SER	1
1	A	292	ASN	1
1	A	301	ASP	1
1	A	210	LYS	1
1	A	294	LYS	1
1	A	245	SER	1
1	A	206	LYS	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 15% for the well-defined parts and 15% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mqe\_cs.str

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

#### 7.1.1 Bookkeeping [i](#)

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	254
Number of shifts mapped to atoms	254
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	—
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	127	$0.13 \pm 0.35$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 15%, i.e. 238 atoms were assigned a chemical shift out of a possible 1539. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	238/630 (38%)	119/251 (47%)	0/256 (0%)	119/123 (97%)
Sidechain	0/842 (0%)	0/491 (0%)	0/306 (0%)	0/45 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/67 (0%)	0/35 (0%)	0/30 (0%)	0/2 (0%)
Overall	238/1539 (15%)	119/777 (15%)	0/592 (0%)	119/170 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 254 atoms were assigned a chemical shift out of a possible 1727. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	254/710 (36%)	127/282 (45%)	0/292 (0%)	127/136 (93%)
Sidechain	0/950 (0%)	0/555 (0%)	0/348 (0%)	0/47 (0%)
Aromatic	0/67 (0%)	0/35 (0%)	0/30 (0%)	0/2 (0%)
Overall	254/1727 (15%)	127/872 (15%)	0/670 (0%)	127/185 (69%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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:

