



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2022 – 03:36 PM EST

PDB ID : 2GZO  
Title : NMR structure of UPF0301 PROTEIN SO3346 from *Shewanella oneidensis*: Northeast Structural Genomics Consortium target SOR39  
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Deposited on : 2006-05-11

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.27  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

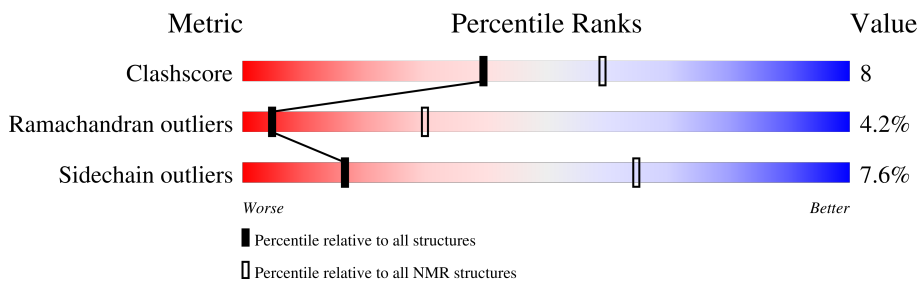
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	195	 66% 13% 16% •

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 20 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:4-A:55, A:70-A:172 (155)	1.23	20

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2866 atoms, of which 1411 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UPF0301 protein SO3346.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	187	2866	917	1411	246	284	8	0

There are 8 discrepancies between the modelled and reference sequences:

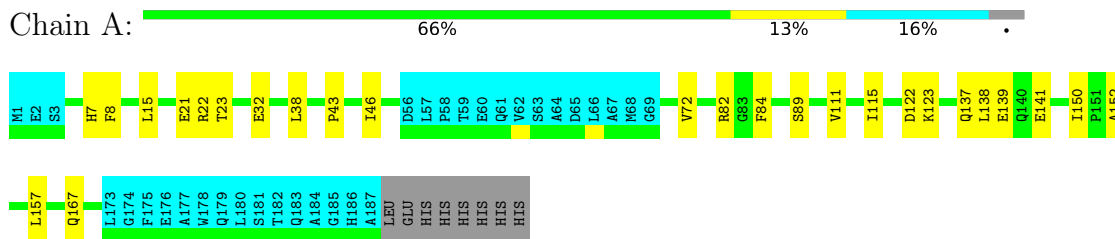
Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	-	expression tag	UNP Q8EBZ9
A	189	GLU	-	expression tag	UNP Q8EBZ9
A	190	HIS	-	expression tag	UNP Q8EBZ9
A	191	HIS	-	expression tag	UNP Q8EBZ9
A	192	HIS	-	expression tag	UNP Q8EBZ9
A	193	HIS	-	expression tag	UNP Q8EBZ9
A	194	HIS	-	expression tag	UNP Q8EBZ9
A	195	HIS	-	expression tag	UNP Q8EBZ9

## 4 Residue-property plots

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

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: UPF0301 protein SO3346

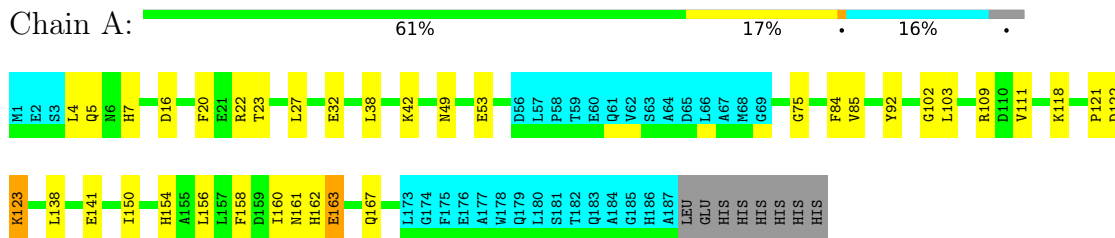


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

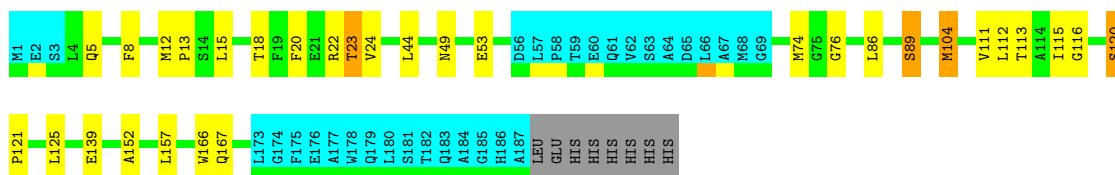
- Molecule 1: UPF0301 protein SO3346



#### 4.2.2 Score per residue for model 2

- Molecule 1: UPF0301 protein SO3346

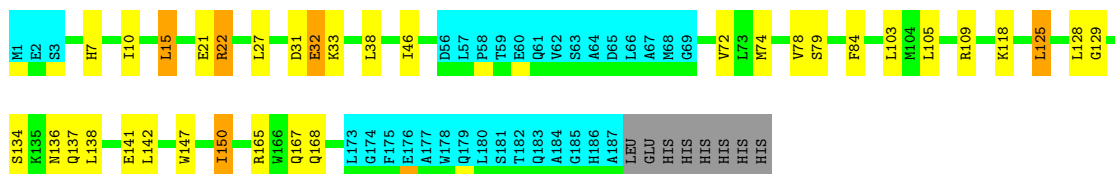




### 4.2.3 Score per residue for model 3

- Molecule 1: UPF0301 protein SO3346

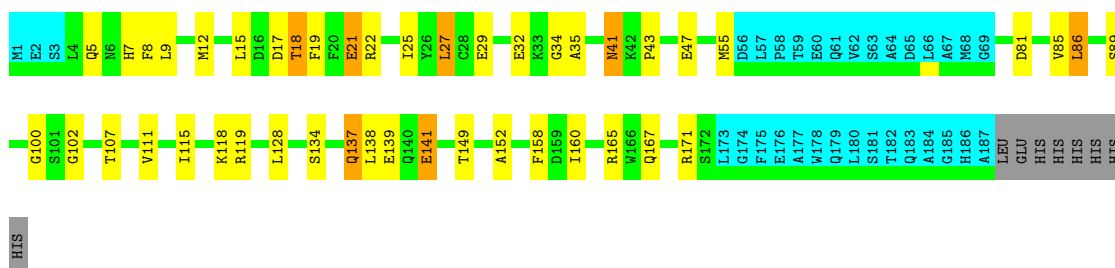
Chain A: 62% 15% 16%



### 4.2.4 Score per residue for model 4

- Molecule 1: UPF0301 protein SO3346

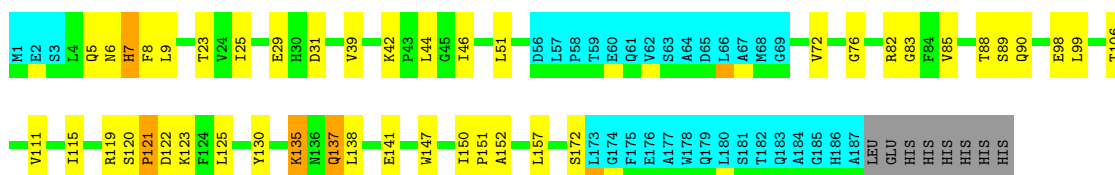
Chain A: 56% 19% 16%



### 4.2.5 Score per residue for model 5

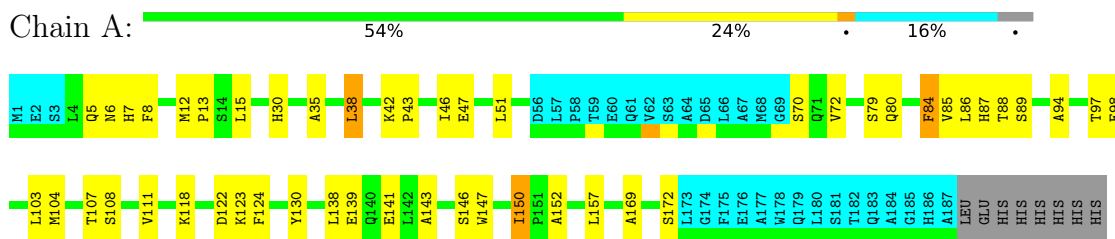
- Molecule 1: UPF0301 protein SO3346

Chain A: 57% 21% 16%



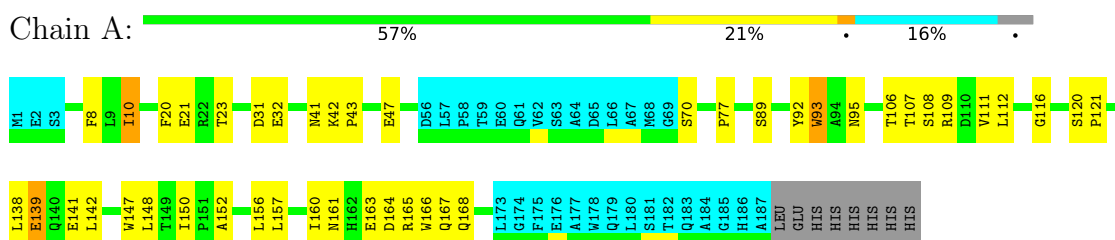
### 4.2.6 Score per residue for model 6

- Molecule 1: UPF0301 protein SO3346



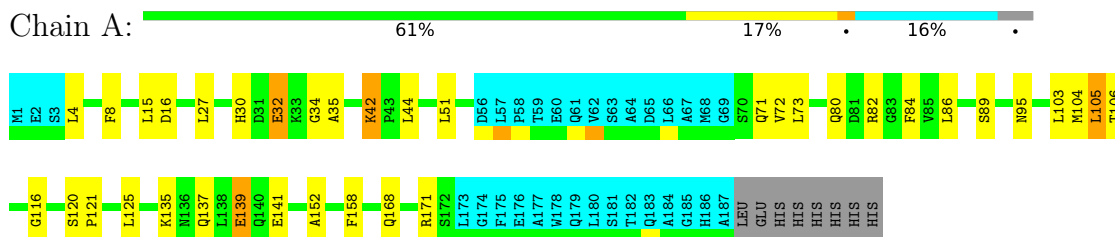
### 4.2.7 Score per residue for model 7

- Molecule 1: UPF0301 protein SO3346



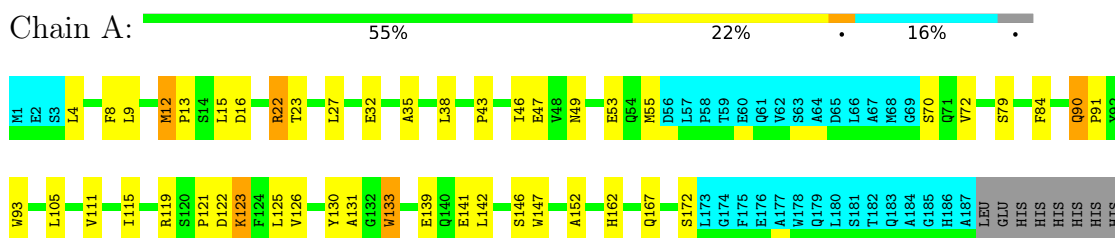
### 4.2.8 Score per residue for model 8

- Molecule 1: UPF0301 protein SO3346



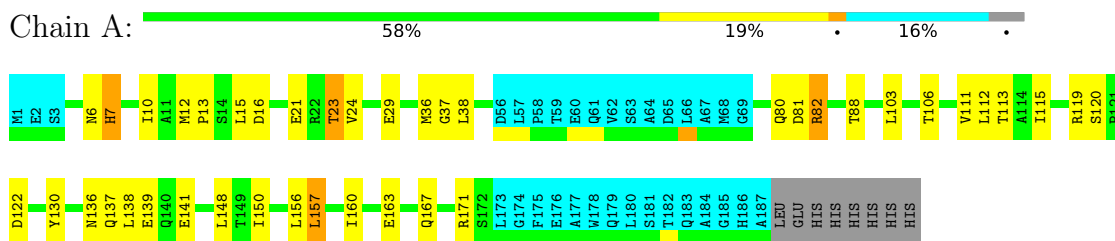
### 4.2.9 Score per residue for model 9

- Molecule 1: UPF0301 protein SO3346



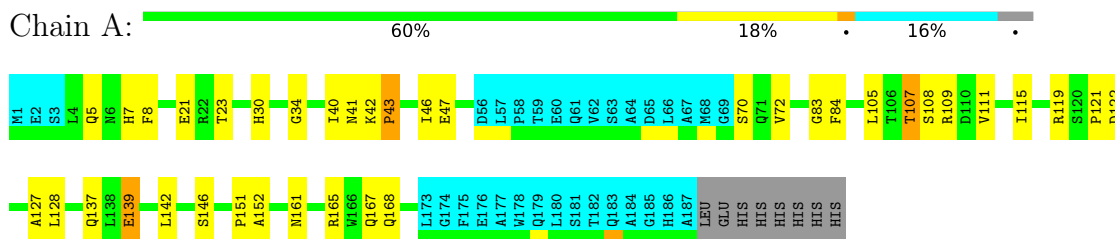
#### 4.2.10 Score per residue for model 10

- Molecule 1: UPF0301 protein SO3346



#### 4.2.11 Score per residue for model 11

- Molecule 1: UPF0301 protein SO3346



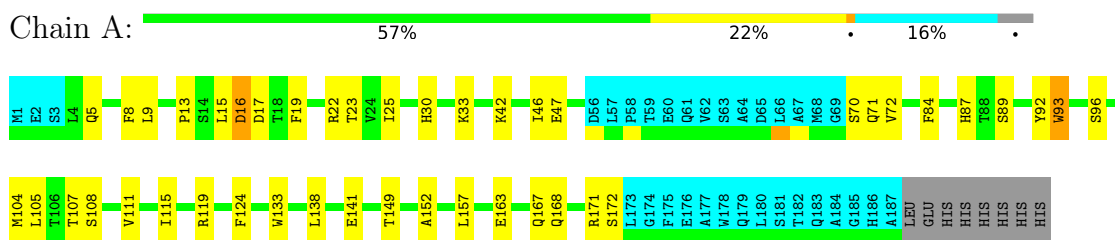
#### 4.2.12 Score per residue for model 12

- Molecule 1: UPF0301 protein SO3346



#### 4.2.13 Score per residue for model 13

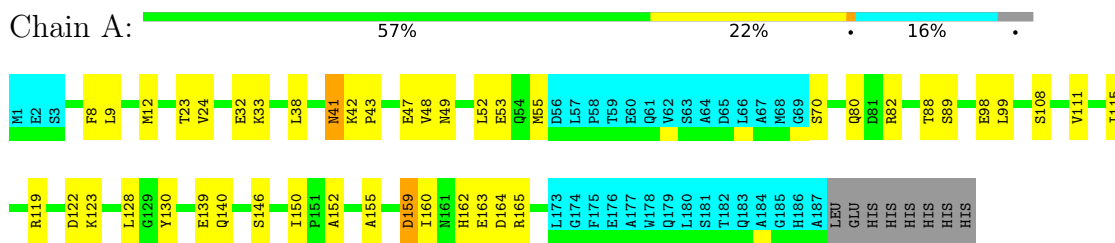
- Molecule 1: UPF0301 protein SO3346





#### 4.2.14 Score per residue for model 14

- Molecule 1: UPF0301 protein SO3346



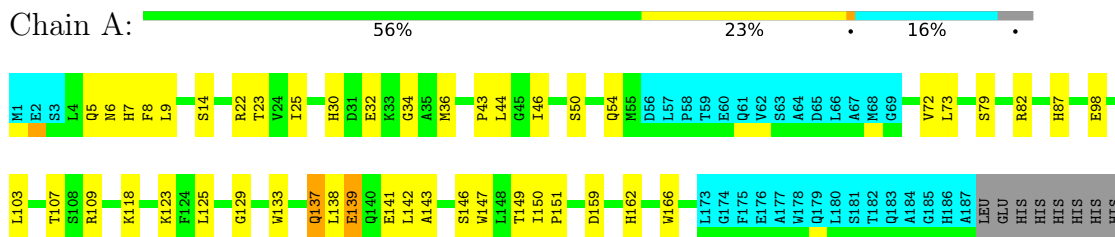
#### 4.2.15 Score per residue for model 15

- Molecule 1: UPF0301 protein SO3346



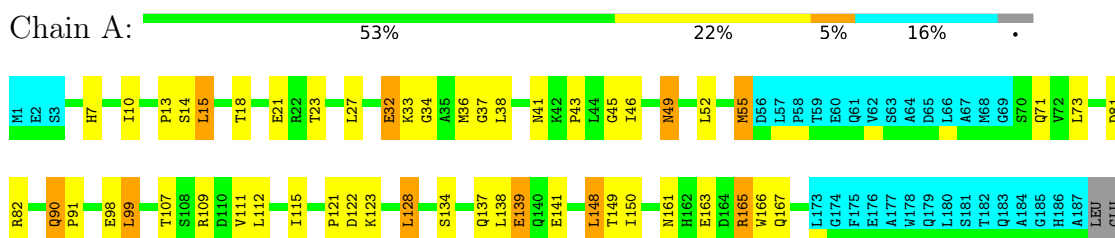
#### 4.2.16 Score per residue for model 16

- Molecule 1: UPF0301 protein SO3346



#### 4.2.17 Score per residue for model 17

- Molecule 1: UPF0301 protein SO3346





## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CYANA	refinement	2.1
CNS	refinement	1.1

No chemical shift data was provided.

## 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	1219	1193	1188	19±4
All	All	24380	23860	23760	373

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LYS:HE3	1:A:118:LYS:HA	0.79	1.51	18	1
1:A:82:ARG:HG2	1:A:109:ARG:HD2	0.79	1.54	16	1
1:A:23:THR:HG21	1:A:41:ASN:HB2	0.79	1.52	17	2
1:A:161:ASN:HA	1:A:165:ARG:HG2	0.78	1.55	17	2
1:A:38:LEU:HG	1:A:75:GLY:HA3	0.76	1.58	1	1
1:A:133:TRP:HB3	1:A:138:LEU:HB3	0.76	1.57	20	1
1:A:134:SER:HA	1:A:138:LEU:HA	0.75	1.57	17	3
1:A:46:ILE:HB	1:A:72:VAL:HB	0.75	1.55	3	10
1:A:45:GLY:HA2	1:A:71:GLN:HA	0.74	1.60	17	1
1:A:21:GLU:HG2	1:A:22:ARG:H	0.73	1.42	15	1
1:A:47:GLU:HA	1:A:70:SER:HA	0.72	1.61	14	5
1:A:160:ILE:HG22	1:A:165:ARG:HG3	0.71	1.61	12	1
1:A:90:GLN:HG3	1:A:91:PRO:HD2	0.71	1.63	12	1
1:A:103:LEU:HG	1:A:154:HIS:HD2	0.70	1.46	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:SER:HB2	1:A:129:GLY:HA2	0.70	1.61	16	2
1:A:51:LEU:HD21	1:A:72:VAL:HG21	0.69	1.65	15	2
1:A:4:LEU:HB3	1:A:27:LEU:HD13	0.68	1.66	18	1
1:A:51:LEU:HD11	1:A:72:VAL:HG21	0.67	1.66	5	2
1:A:4:LEU:HA	1:A:7:HIS:HE1	0.66	1.50	1	1
1:A:46:ILE:HD11	1:A:74:MET:HB2	0.66	1.68	3	2
1:A:143:ALA:HA	1:A:147:TRP:HB2	0.66	1.68	6	1
1:A:120:SER:HB2	1:A:124:PHE:HD2	0.66	1.51	18	1
1:A:10:ILE:HB	1:A:148:LEU:HB2	0.65	1.67	12	2
1:A:139:GLU:HA	1:A:142:LEU:HD12	0.65	1.68	11	1
1:A:137:GLN:HB3	1:A:141:GLU:HB3	0.65	1.66	3	3
1:A:34:GLY:HA3	1:A:139:GLU:HG3	0.64	1.67	8	1
1:A:84:PHE:HB3	1:A:107:THR:HG22	0.64	1.69	13	2
1:A:8:PHE:CE2	1:A:152:ALA:HA	0.63	2.28	20	12
1:A:85:VAL:HB	1:A:111:VAL:HG21	0.63	1.69	15	4
1:A:138:LEU:O	1:A:141:GLU:HG2	0.63	1.93	6	8
1:A:7:HIS:HB2	1:A:150:ILE:O	0.63	1.93	1	7
1:A:13:PRO:HA	1:A:17:ASP:OD2	0.63	1.94	13	1
1:A:139:GLU:O	1:A:142:LEU:HG	0.62	1.94	20	2
1:A:120:SER:HB2	1:A:121:PRO:HD3	0.62	1.72	2	1
1:A:95:ASN:HB2	1:A:106:THR:HG23	0.62	1.72	15	2
1:A:22:ARG:HG2	1:A:23:THR:H	0.62	1.55	18	2
1:A:18:THR:HG23	1:A:19:PHE:H	0.60	1.56	4	1
1:A:34:GLY:HA2	1:A:139:GLU:HG2	0.60	1.73	11	1
1:A:6:ASN:HB2	1:A:99:LEU:HD12	0.59	1.74	5	1
1:A:6:ASN:HA	1:A:27:LEU:O	0.59	1.96	15	1
1:A:4:LEU:HA	1:A:7:HIS:CE1	0.59	2.31	1	1
1:A:109:ARG:HA	1:A:112:LEU:HD13	0.59	1.75	19	1
1:A:135:LYS:HE3	1:A:135:LYS:HA	0.58	1.73	5	1
1:A:82:ARG:HG2	1:A:83:GLY:H	0.58	1.56	5	1
1:A:137:GLN:HB3	1:A:141:GLU:OE1	0.58	1.98	16	1
1:A:47:GLU:HA	1:A:70:SER:H	0.58	1.57	11	1
1:A:7:HIS:HD2	1:A:151:PRO:HA	0.58	1.58	11	2
1:A:4:LEU:HB3	1:A:7:HIS:HE1	0.58	1.58	12	1
1:A:86:LEU:HB3	1:A:158:PHE:HZ	0.57	1.59	8	1
1:A:29:GLU:HB2	1:A:36:MET:HB2	0.57	1.75	10	1
1:A:44:LEU:HG	1:A:74:MET:HG2	0.57	1.76	2	1
1:A:73:LEU:HD12	1:A:125:LEU:HD21	0.56	1.77	16	1
1:A:155:ALA:HA	1:A:159:ASP:HB3	0.56	1.75	18	2
1:A:8:PHE:HB2	1:A:150:ILE:HG13	0.56	1.76	5	4
1:A:150:ILE:HG13	1:A:169:ALA:HB1	0.56	1.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:GLN:HG3	1:A:30:HIS:HB3	0.56	1.77	13	1
1:A:22:ARG:HD2	1:A:23:THR:H	0.56	1.60	13	1
1:A:15:LEU:HD21	1:A:21:GLU:HB2	0.55	1.77	10	1
1:A:120:SER:HB2	1:A:124:PHE:CD2	0.55	2.36	18	1
1:A:9:LEU:HB2	1:A:25:ILE:HB	0.55	1.78	16	3
1:A:160:ILE:O	1:A:165:ARG:HD3	0.55	2.01	14	3
1:A:136:ASN:HB2	1:A:141:GLU:OE2	0.55	2.02	10	1
1:A:49:ASN:O	1:A:53:GLU:HG3	0.55	2.02	14	4
1:A:23:THR:HG23	1:A:166:TRP:CZ3	0.55	2.36	2	1
1:A:111:VAL:HG13	1:A:112:LEU:HD22	0.54	1.78	10	3
1:A:52:LEU:HA	1:A:55:MET:CG	0.54	2.32	17	1
1:A:22:ARG:HH11	1:A:22:ARG:HB3	0.54	1.61	16	1
1:A:111:VAL:O	1:A:115:ILE:HG13	0.53	2.03	12	12
1:A:12:MET:HB2	1:A:13:PRO:HD3	0.53	1.80	20	3
1:A:89:SER:HA	1:A:104:MET:SD	0.53	2.44	2	1
1:A:43:PRO:HA	1:A:73:LEU:CD2	0.53	2.33	17	1
1:A:22:ARG:O	1:A:23:THR:HG22	0.53	2.03	1	1
1:A:23:THR:HG22	1:A:24:VAL:HG23	0.53	1.81	2	3
1:A:90:GLN:CB	1:A:91:PRO:HD3	0.53	2.34	9	1
1:A:134:SER:HA	1:A:138:LEU:CA	0.52	2.33	17	1
1:A:38:LEU:HD23	1:A:84:PHE:HE1	0.52	1.65	6	1
1:A:136:ASN:O	1:A:137:GLN:HB2	0.52	2.04	20	1
1:A:8:PHE:O	1:A:149:THR:HA	0.52	2.04	16	3
1:A:52:LEU:HA	1:A:55:MET:HG3	0.52	1.80	17	1
1:A:4:LEU:O	1:A:35:ALA:HB2	0.51	2.05	9	2
1:A:81:ASP:OD2	1:A:82:ARG:HD2	0.51	2.04	10	1
1:A:133:TRP:CD1	1:A:139:GLU:HA	0.51	2.40	16	1
1:A:138:LEU:O	1:A:141:GLU:HG3	0.51	2.05	13	2
1:A:96:SER:HB3	1:A:104:MET:SD	0.51	2.46	20	1
1:A:12:MET:O	1:A:15:LEU:HG	0.51	2.05	4	1
1:A:5:GLN:OE1	1:A:30:HIS:HB2	0.51	2.05	11	1
1:A:120:SER:H	1:A:121:PRO:HD2	0.51	1.66	7	1
1:A:33:LYS:HD3	1:A:137:GLN:HG2	0.51	1.81	12	1
1:A:97:THR:HB	1:A:105:LEU:HB2	0.51	1.82	15	1
1:A:136:ASN:HB2	1:A:141:GLU:OE1	0.51	2.06	3	1
1:A:76:GLY:O	1:A:129:GLY:HA3	0.51	2.05	12	1
1:A:42:LYS:HD3	1:A:71:GLN:HE22	0.51	1.65	13	1
1:A:87:HIS:O	1:A:103:LEU:HB2	0.50	2.06	6	1
1:A:156:LEU:HD23	1:A:160:ILE:HD12	0.50	1.81	10	2
1:A:36:MET:HA	1:A:133:TRP:CZ3	0.50	2.42	16	1
1:A:93:TRP:HZ2	1:A:110:ASP:HB3	0.50	1.66	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HB3	1:A:7:HIS:CE1	0.50	2.41	12	1
1:A:120:SER:N	1:A:121:PRO:HD2	0.50	2.22	7	1
1:A:41:ASN:HA	1:A:165:ARG:NH2	0.50	2.21	4	1
1:A:6:ASN:O	1:A:7:HIS:HB2	0.50	2.07	10	3
1:A:23:THR:HA	1:A:166:TRP:CZ3	0.50	2.41	17	1
1:A:163:GLU:CD	1:A:163:GLU:H	0.50	2.09	1	1
1:A:142:LEU:HD12	1:A:143:ALA:N	0.49	2.22	16	1
1:A:106:THR:CG2	1:A:111:VAL:HB	0.49	2.37	15	2
1:A:122:ASP:OD2	1:A:123:LYS:HG2	0.49	2.07	14	5
1:A:106:THR:HB	1:A:111:VAL:HB	0.49	1.83	18	1
1:A:4:LEU:O	1:A:5:GLN:HB3	0.49	2.07	1	1
1:A:103:LEU:HD12	1:A:157:LEU:HD13	0.49	1.83	10	1
1:A:9:LEU:O	1:A:24:VAL:HA	0.49	2.07	14	2
1:A:93:TRP:HE1	1:A:106:THR:HG21	0.48	1.68	15	1
1:A:128:LEU:O	1:A:128:LEU:HD12	0.48	2.09	14	1
1:A:5:GLN:HG3	1:A:30:HIS:HB2	0.48	1.84	16	1
1:A:49:ASN:O	1:A:52:LEU:HG	0.48	2.09	17	2
1:A:78:VAL:O	1:A:129:GLY:HA3	0.48	2.09	18	1
1:A:15:LEU:HD23	1:A:146:SER:HB2	0.48	1.86	6	1
1:A:38:LEU:HD12	1:A:84:PHE:CE2	0.48	2.44	15	3
1:A:84:PHE:HA	1:A:107:THR:CG2	0.48	2.38	11	1
1:A:111:VAL:O	1:A:115:ILE:HG12	0.47	2.09	4	1
1:A:12:MET:H	1:A:13:PRO:HD2	0.47	1.69	6	1
1:A:92:TYR:CG	1:A:93:TRP:N	0.47	2.83	15	2
1:A:84:PHE:CD1	1:A:105:LEU:HD21	0.47	2.44	9	2
1:A:55:MET:CE	1:A:55:MET:HA	0.47	2.40	9	1
1:A:159:ASP:OD1	1:A:162:HIS:HA	0.47	2.09	15	1
1:A:82:ARG:HB3	1:A:130:TYR:HE2	0.47	1.70	5	1
1:A:15:LEU:HD22	1:A:15:LEU:N	0.46	2.24	18	3
1:A:54:GLN:HG2	1:A:109:ARG:NH2	0.46	2.24	19	1
1:A:161:ASN:O	1:A:162:HIS:HB2	0.46	2.10	20	1
1:A:142:LEU:HG	1:A:147:TRP:CD1	0.46	2.46	7	1
1:A:137:GLN:O	1:A:138:LEU:HG	0.46	2.10	17	1
1:A:110:ASP:O	1:A:113:THR:HG22	0.46	2.11	18	1
1:A:22:ARG:HD2	1:A:23:THR:N	0.46	2.24	13	1
1:A:8:PHE:HB2	1:A:150:ILE:CG1	0.46	2.41	14	2
1:A:21:GLU:CD	1:A:22:ARG:HD2	0.46	2.31	4	1
1:A:50:SER:O	1:A:54:GLN:HG3	0.46	2.10	16	1
1:A:161:ASN:HA	1:A:165:ARG:CG	0.46	2.37	17	1
1:A:109:ARG:C	1:A:109:ARG:HD2	0.46	2.31	3	1
1:A:32:GLU:HG3	1:A:33:LYS:H	0.46	1.71	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:GLU:HA	1:A:147:TRP:HZ2	0.46	1.71	3	1
1:A:34:GLY:HA3	1:A:139:GLU:HB3	0.46	1.87	4	1
1:A:30:HIS:HA	1:A:35:ALA:HA	0.46	1.88	8	3
1:A:22:ARG:HD3	1:A:22:ARG:N	0.46	2.26	9	1
1:A:83:GLY:HA3	1:A:127:ALA:O	0.46	2.11	11	1
1:A:122:ASP:OD2	1:A:123:LYS:HG3	0.45	2.11	1	1
1:A:27:LEU:HA	1:A:37:GLY:CA	0.45	2.42	17	1
1:A:155:ALA:HA	1:A:159:ASP:CB	0.45	2.41	18	1
1:A:38:LEU:HD23	1:A:84:PHE:CE1	0.45	2.47	6	1
1:A:84:PHE:HZ	1:A:130:TYR:HB3	0.45	1.71	6	1
1:A:12:MET:HB3	1:A:13:PRO:HD3	0.45	1.89	9	2
1:A:85:VAL:HG13	1:A:125:LEU:O	0.45	2.11	5	2
1:A:90:GLN:HE21	1:A:91:PRO:HD2	0.45	1.71	17	1
1:A:8:PHE:HZ	1:A:157:LEU:HG	0.45	1.71	5	1
1:A:90:GLN:CG	1:A:91:PRO:HD2	0.45	2.40	12	1
1:A:162:HIS:O	1:A:164:ASP:N	0.45	2.50	14	1
1:A:10:ILE:HB	1:A:148:LEU:HB3	0.45	1.87	17	1
1:A:111:VAL:HG13	1:A:112:LEU:HD12	0.45	1.87	19	2
1:A:15:LEU:HD12	1:A:16:ASP:N	0.45	2.27	13	1
1:A:52:LEU:HD12	1:A:53:GLU:N	0.45	2.27	18	1
1:A:73:LEU:HD12	1:A:125:LEU:HD11	0.45	1.89	8	1
1:A:23:THR:HA	1:A:166:TRP:HZ3	0.44	1.73	16	1
1:A:109:ARG:HA	1:A:112:LEU:HD23	0.44	1.88	17	1
1:A:150:ILE:HD12	1:A:169:ALA:HB1	0.44	1.88	19	1
1:A:97:THR:O	1:A:104:MET:HA	0.44	2.12	6	1
1:A:9:LEU:HB3	1:A:147:TRP:CE3	0.44	2.47	16	2
1:A:7:HIS:HB3	1:A:150:ILE:O	0.44	2.11	16	1
1:A:93:TRP:CZ2	1:A:119:ARG:HG2	0.44	2.47	9	1
1:A:22:ARG:O	1:A:22:ARG:HD2	0.44	2.12	3	1
1:A:155:ALA:HA	1:A:159:ASP:HB2	0.44	1.88	14	1
1:A:119:ARG:HG3	1:A:120:SER:H	0.44	1.71	10	1
1:A:150:ILE:N	1:A:150:ILE:HD13	0.44	2.27	6	1
1:A:103:LEU:HD13	1:A:158:PHE:HE2	0.44	1.73	8	2
1:A:27:LEU:HD21	1:A:133:TRP:CZ2	0.44	2.48	9	1
1:A:90:GLN:HE21	1:A:90:GLN:HA	0.44	1.73	17	1
1:A:148:LEU:HD13	1:A:149:THR:N	0.44	2.28	17	1
1:A:118:LYS:HA	1:A:118:LYS:CE	0.44	2.36	18	1
1:A:22:ARG:CD	1:A:23:THR:H	0.43	2.26	13	1
1:A:99:LEU:N	1:A:99:LEU:HD13	0.43	2.28	17	1
1:A:95:ASN:OD1	1:A:106:THR:HA	0.43	2.14	8	1
1:A:108:SER:O	1:A:111:VAL:HG12	0.43	2.12	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:HIS:O	1:A:103:LEU:HB3	0.43	2.14	16	1
1:A:29:GLU:O	1:A:35:ALA:HB1	0.43	2.14	4	1
1:A:90:GLN:HG2	1:A:121:PRO:HB3	0.43	1.89	5	1
1:A:103:LEU:HD21	1:A:157:LEU:HD13	0.43	1.91	15	2
1:A:22:ARG:HA	1:A:147:TRP:HH2	0.43	1.73	15	1
1:A:15:LEU:HD12	1:A:18:THR:HG23	0.43	1.89	17	1
1:A:87:HIS:CD2	1:A:124:PHE:HB3	0.43	2.48	6	1
1:A:34:GLY:HA2	1:A:139:GLU:HG3	0.43	1.89	17	1
1:A:23:THR:HA	1:A:166:TRP:CH2	0.43	2.48	18	2
1:A:164:ASP:OD2	1:A:168:GLN:HG3	0.43	2.14	7	1
1:A:92:TYR:O	1:A:93:TRP:HB2	0.43	2.13	13	1
1:A:37:GLY:O	1:A:130:TYR:HB2	0.43	2.14	10	1
1:A:7:HIS:CD2	1:A:151:PRO:HA	0.43	2.49	16	1
1:A:134:SER:HA	1:A:139:GLU:OE2	0.43	2.13	19	1
1:A:26:TYR:O	1:A:37:GLY:HA3	0.43	2.14	20	1
1:A:128:LEU:HD12	1:A:128:LEU:O	0.43	2.14	3	5
1:A:168:GLN:O	1:A:171:ARG:HG2	0.43	2.13	8	1
1:A:42:LYS:N	1:A:43:PRO:HD3	0.43	2.28	11	1
1:A:38:LEU:HB2	1:A:84:PHE:CZ	0.43	2.49	1	1
1:A:139:GLU:H	1:A:139:GLU:CD	0.43	2.17	2	1
1:A:55:MET:HA	1:A:55:MET:CE	0.43	2.44	4	1
1:A:25:ILE:HG12	1:A:39:VAL:HG22	0.43	1.91	5	1
1:A:96:SER:HB3	1:A:104:MET:HG2	0.42	1.90	13	1
1:A:20:PHE:HE1	1:A:76:GLY:HA2	0.42	1.72	2	1
1:A:15:LEU:HD12	1:A:21:GLU:HB3	0.42	1.90	3	1
1:A:9:LEU:HB3	1:A:147:TRP:HE3	0.42	1.73	5	2
1:A:22:ARG:HA	1:A:147:TRP:CH2	0.42	2.49	15	1
1:A:86:LEU:O	1:A:124:PHE:HA	0.42	2.15	6	1
1:A:21:GLU:HG2	1:A:22:ARG:N	0.42	2.20	15	1
1:A:5:GLN:HG2	1:A:6:ASN:N	0.42	2.29	20	1
1:A:125:LEU:HD13	1:A:125:LEU:N	0.42	2.30	3	1
1:A:21:GLU:H	1:A:21:GLU:CD	0.42	2.18	7	1
1:A:5:GLN:O	1:A:27:LEU:HB2	0.42	2.15	4	1
1:A:130:TYR:HD1	1:A:131:ALA:O	0.42	1.98	9	1
1:A:95:ASN:HB3	1:A:106:THR:HA	0.41	1.92	15	2
1:A:138:LEU:HG	1:A:139:GLU:OE2	0.41	2.15	7	1
1:A:142:LEU:HA	1:A:147:TRP:CD1	0.41	2.50	7	1
1:A:120:SER:OG	1:A:121:PRO:HD3	0.41	2.14	8	1
1:A:43:PRO:HD2	1:A:73:LEU:HD23	0.41	1.91	19	1
1:A:86:LEU:HD13	1:A:86:LEU:N	0.41	2.30	4	1
1:A:86:LEU:HD23	1:A:158:PHE:CE1	0.41	2.50	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:SER:O	1:A:80:GLN:HB2	0.41	2.15	6	1
1:A:10:ILE:HG13	1:A:148:LEU:HB2	0.41	1.92	7	1
1:A:16:ASP:HA	1:A:22:ARG:NH1	0.41	2.30	1	1
1:A:85:VAL:HG21	1:A:111:VAL:HG11	0.41	1.91	1	1
1:A:27:LEU:O	1:A:27:LEU:HD12	0.41	2.15	3	1
1:A:8:PHE:HB2	1:A:150:ILE:HG12	0.41	1.91	6	1
1:A:137:GLN:HA	1:A:137:GLN:OE1	0.41	2.15	11	1
1:A:5:GLN:HG2	1:A:6:ASN:H	0.41	1.74	20	1
1:A:27:LEU:HD12	1:A:27:LEU:N	0.41	2.31	1	1
1:A:156:LEU:HA	1:A:160:ILE:HD12	0.41	1.92	1	1
1:A:10:ILE:HG12	1:A:150:ILE:HD12	0.41	1.91	3	1
1:A:31:ASP:O	1:A:33:LYS:N	0.41	2.54	3	1
1:A:82:ARG:HB3	1:A:130:TYR:CE2	0.41	2.51	5	1
1:A:4:LEU:HD22	1:A:139:GLU:HB3	0.41	1.92	9	1
1:A:153:ASP:O	1:A:157:LEU:HB2	0.41	2.14	15	1
1:A:15:LEU:N	1:A:15:LEU:HD23	0.41	2.31	17	1
1:A:19:PHE:HA	1:A:22:ARG:NE	0.41	2.31	12	1
1:A:123:LYS:O	1:A:123:LYS:HD3	0.41	2.14	18	1
1:A:21:GLU:HB3	1:A:23:THR:HG22	0.41	1.93	19	1
1:A:86:LEU:HB3	1:A:125:LEU:HD21	0.41	1.92	2	1
1:A:15:LEU:HD22	1:A:15:LEU:H	0.41	1.76	10	1
1:A:87:HIS:HB3	1:A:124:PHE:HB3	0.41	1.93	13	1
1:A:22:ARG:HD2	1:A:22:ARG:N	0.41	2.30	19	1
1:A:28:CYS:SG	1:A:105:LEU:HD21	0.41	2.56	19	1
1:A:12:MET:HG2	1:A:166:TRP:CZ2	0.40	2.51	2	1
1:A:103:LEU:H	1:A:103:LEU:HD23	0.40	1.75	3	1
1:A:137:GLN:HG2	1:A:138:LEU:HG	0.40	1.94	5	1
1:A:5:GLN:HG3	1:A:29:GLU:HA	0.40	1.92	4	1
1:A:125:LEU:HD13	1:A:126:VAL:N	0.40	2.31	9	1
1:A:46:ILE:HD12	1:A:128:LEU:HD21	0.40	1.92	17	1
1:A:98:GLU:O	1:A:99:LEU:HB2	0.40	2.16	18	1
1:A:78:VAL:O	1:A:79:SER:HB2	0.40	2.16	3	1
1:A:44:LEU:HB2	1:A:73:LEU:HD23	0.40	1.94	8	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation

was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/195 (79%)	123±4 (79±3%)	25±4 (16±2%)	7±2 (4±1%)	5	30
All	All	3100/3900 (79%)	2462 (79%)	507 (16%)	131 (4%)	5	30

All 50 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	32	GLU	12
1	A	43	PRO	8
1	A	146	SER	8
1	A	121	PRO	6
1	A	118	LYS	6
1	A	172	SER	5
1	A	16	ASP	5
1	A	23	THR	4
1	A	42	LYS	4
1	A	137	GLN	4
1	A	108	SER	4
1	A	122	ASP	4
1	A	20	PHE	3
1	A	109	ARG	3
1	A	161	ASN	3
1	A	18	THR	3
1	A	120	SER	3
1	A	41	ASN	3
1	A	82	ARG	3
1	A	40	ILE	3
1	A	162	HIS	3
1	A	102	GLY	2
1	A	165	ARG	2
1	A	31	ASP	2
1	A	163	GLU	2
1	A	14	SER	2
1	A	15	LEU	1
1	A	17	ASP	1
1	A	100	GLY	1
1	A	119	ARG	1
1	A	5	GLN	1
1	A	7	HIS	1
1	A	76	GLY	1
1	A	6	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	94	ALA	1
1	A	77	PRO	1
1	A	80	GLN	1
1	A	12	MET	1
1	A	79	SER	1
1	A	90	GLN	1
1	A	91	PRO	1
1	A	19	PHE	1
1	A	93	TRP	1
1	A	4	LEU	1
1	A	22	ARG	1
1	A	159	ASP	1
1	A	34	GLY	1
1	A	13	PRO	1
1	A	81	ASP	1
1	A	138	LEU	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	134/166 (81%)	124±3 (92±2%)	10±3 (8±2%)	17 65
All	All	2680/3320 (81%)	2476 (92%)	204 (8%)	17 65

All 71 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	167	GLN	12
1	A	89	SER	11
1	A	157	LEU	10
1	A	139	GLU	8
1	A	163	GLU	7
1	A	107	THR	7
1	A	38	LEU	7
1	A	88	THR	6
1	A	123	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	105	LEU	5
1	A	150	ILE	5
1	A	21	GLU	5
1	A	141	GLU	5
1	A	23	THR	5
1	A	98	GLU	5
1	A	119	ARG	5
1	A	82	ARG	5
1	A	42	LYS	4
1	A	104	MET	4
1	A	15	LEU	4
1	A	168	GLN	4
1	A	118	LYS	3
1	A	162	HIS	3
1	A	171	ARG	3
1	A	29	GLU	3
1	A	135	LYS	3
1	A	133	TRP	3
1	A	112	LEU	2
1	A	22	ARG	2
1	A	32	GLU	2
1	A	7	HIS	2
1	A	27	LEU	2
1	A	44	LEU	2
1	A	84	PHE	2
1	A	80	GLN	2
1	A	165	ARG	2
1	A	33	LYS	2
1	A	55	MET	2
1	A	99	LEU	2
1	A	159	ASP	2
1	A	92	TYR	1
1	A	158	PHE	1
1	A	125	LEU	1
1	A	142	LEU	1
1	A	47	GLU	1
1	A	81	ASP	1
1	A	86	LEU	1
1	A	137	GLN	1
1	A	5	GLN	1
1	A	10	ILE	1
1	A	93	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	71	GLN	1
1	A	106	THR	1
1	A	41	ASN	1
1	A	122	ASP	1
1	A	161	ASN	1
1	A	12	MET	1
1	A	130	TYR	1
1	A	140	GLN	1
1	A	40	ILE	1
1	A	36	MET	1
1	A	49	ASN	1
1	A	90	GLN	1
1	A	128	LEU	1
1	A	148	LEU	1
1	A	30	HIS	1
1	A	124	PHE	1
1	A	138	LEU	1
1	A	97	THR	1
1	A	103	LEU	1
1	A	170	SER	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided