



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2022 – 12:11 am GMT

PDB ID : 7QI2  
Title : Magic-angle spinning NMR structure of the human voltage-dependent anion channel 1 (E73V/C127A/C232S) in DMPC lipid bilayers  
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Deposited on : 2021-12-14

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

<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

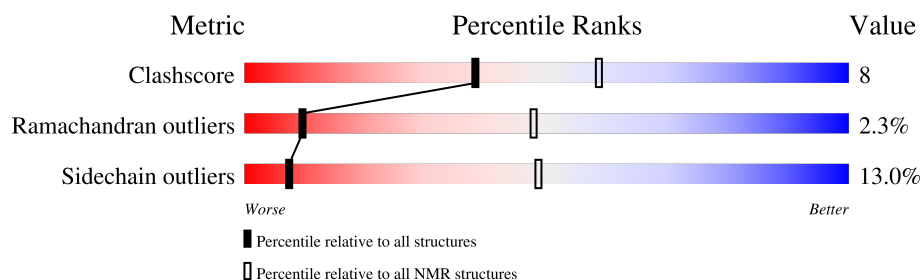
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 35%.

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	291	 67% 12% 19% .

## 2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:14-A:15, A:24-A:33, A:37-A:48, A:52-A:102, A:110-A:156, A:167-A:251, A:255-A:265, A:273-A:283 (229)	1.80	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4313 atoms, of which 2146 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Voltage-dependent anion-selective channel protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	283	Total	C	H	N	O	S	0
			4313	1372	2146	366	426	3	

There are 11 discrepancies between the modelled and reference sequences:

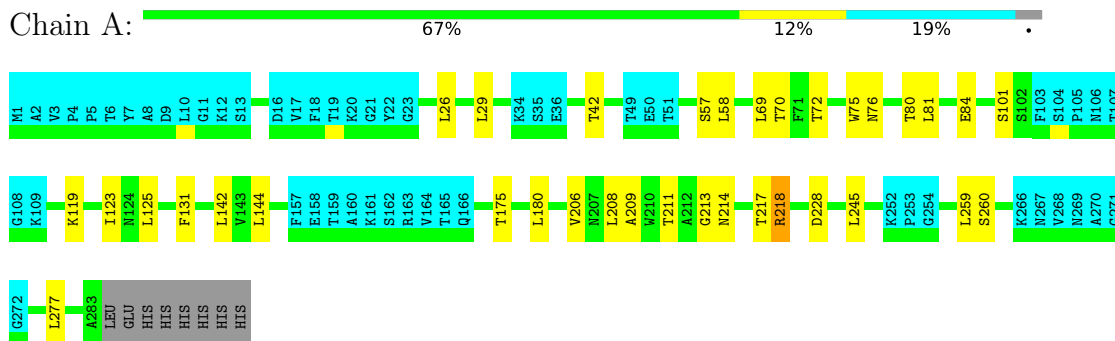
Chain	Residue	Modelled	Actual	Comment	Reference
A	73	VAL	GLU	engineered mutation	UNP P21796
A	127	ALA	CYS	engineered mutation	UNP P21796
A	232	SER	CYS	engineered mutation	UNP P21796
A	284	LEU	-	expression tag	UNP P21796
A	285	GLU	-	expression tag	UNP P21796
A	286	HIS	-	expression tag	UNP P21796
A	287	HIS	-	expression tag	UNP P21796
A	288	HIS	-	expression tag	UNP P21796
A	289	HIS	-	expression tag	UNP P21796
A	290	HIS	-	expression tag	UNP P21796
A	291	HIS	-	expression tag	UNP P21796

## 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: Voltage-dependent anion-selective channel protein 1

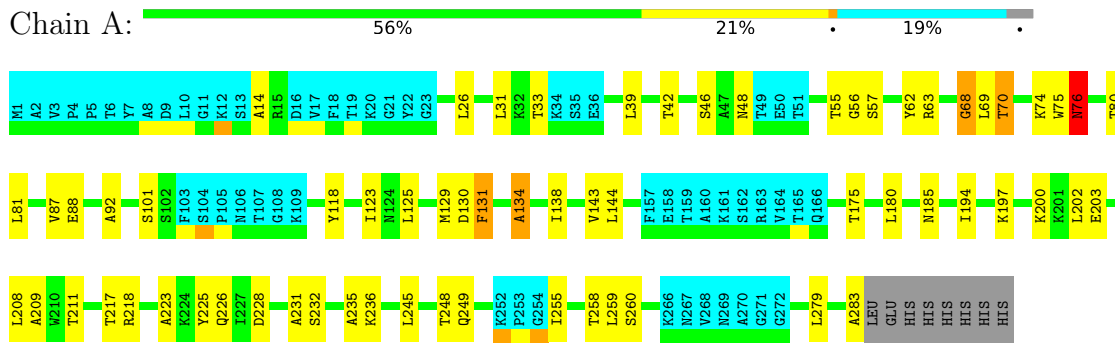


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

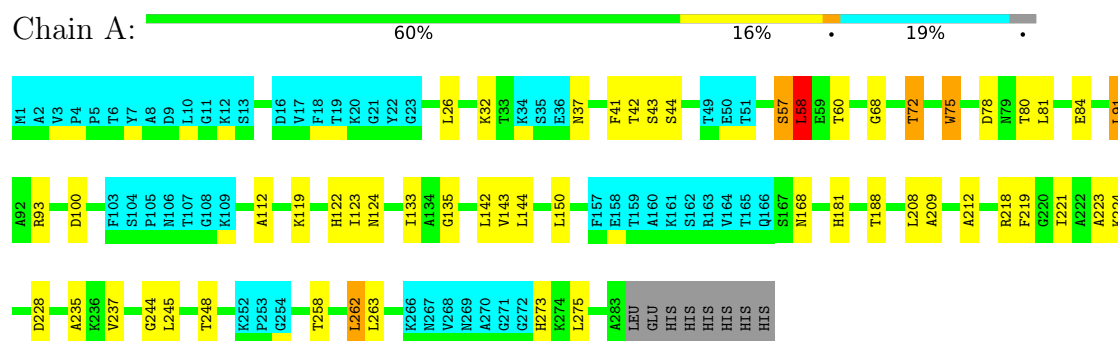
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Voltage-dependent anion-selective channel protein 1



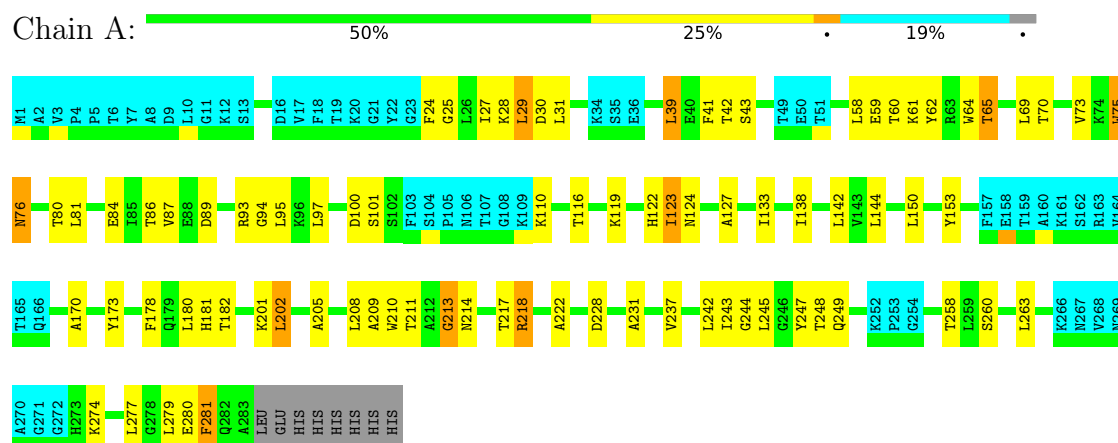
### 4.2.2 Score per residue for model 2

- Molecule 1: Voltage-dependent anion-selective channel protein 1



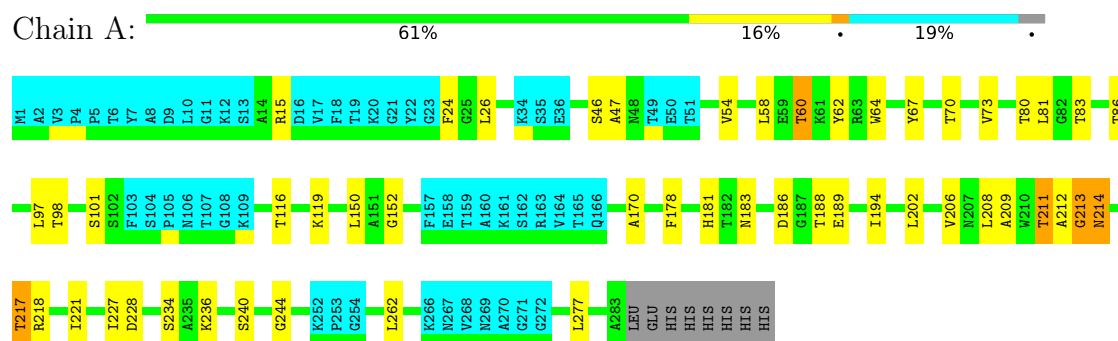
### 4.2.5 Score per residue for model 5

- Molecule 1: Voltage-dependent anion-selective channel protein 1



### 4.2.6 Score per residue for model 6

- Molecule 1: Voltage-dependent anion-selective channel protein 1



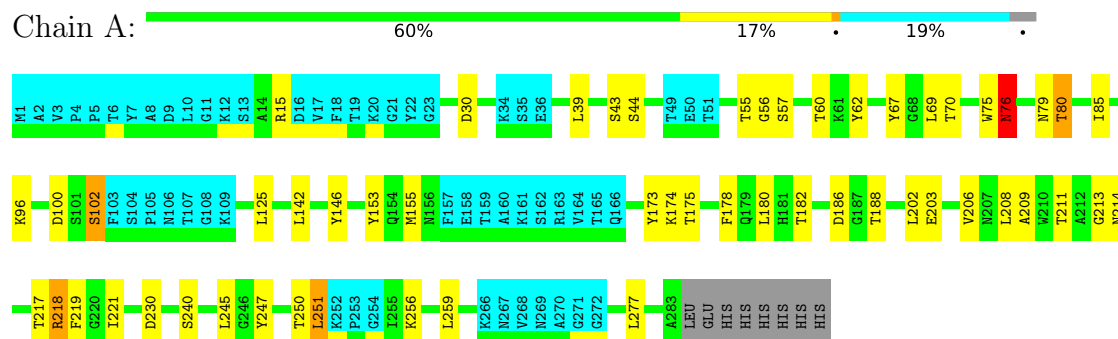
### 4.2.7 Score per residue for model 7

- Molecule 1: Voltage-dependent anion-selective channel protein 1



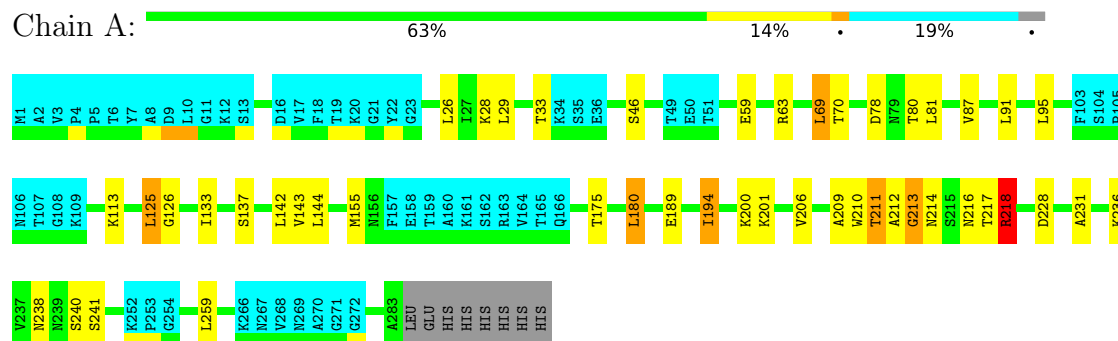
### 4.2.8 Score per residue for model 8

- Molecule 1: Voltage-dependent anion-selective channel protein 1



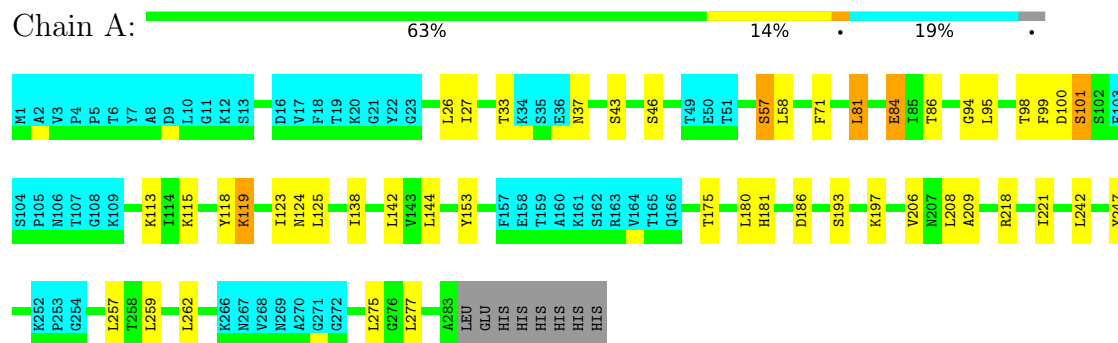
### 4.2.9 Score per residue for model 9

- Molecule 1: Voltage-dependent anion-selective channel protein 1



### 4.2.10 Score per residue for model 10

- Molecule 1: Voltage-dependent anion-selective channel protein 1





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 2400 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.13

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1056
Number of shifts mapped to atoms	1056
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 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	1767	1751	1751	28±6
All	All	17670	17510	17510	283

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:206:VAL:HG12	1:A:221:ILE:HG23	1.00	1.31	6	2
1:A:223:ALA:HB3	1:A:235:ALA:HB3	0.99	1.29	2	3
1:A:212:ALA:O	1:A:214:ASN:N	0.94	2.01	9	2
1:A:248:THR:HG23	1:A:258:THR:HG22	0.83	1.48	1	1
1:A:205:ALA:HB3	1:A:222:ALA:HB3	0.81	1.51	3	1
1:A:69:LEU:HD11	1:A:87:VAL:HG12	0.81	1.52	5	1
1:A:47:ALA:HB2	1:A:54:VAL:HG23	0.74	1.58	6	1
1:A:84:GLU:HB3	1:A:99:PHE:O	0.74	1.83	10	1
1:A:242:LEU:HD13	1:A:262:LEU:HD11	0.72	1.61	10	1
1:A:86:THR:HG23	1:A:98:THR:HG22	0.71	1.62	10	1
1:A:242:LEU:HD21	1:A:262:LEU:HD21	0.69	1.65	4	1
1:A:180:LEU:HD22	1:A:180:LEU:C	0.68	2.09	9	1
1:A:245:LEU:HD21	1:A:261:ALA:HB3	0.68	1.64	7	1
1:A:76:ASN:O	1:A:77:THR:C	0.65	2.34	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:ILE:HD12	1:A:144:LEU:HD12	0.65	1.68	10	1
1:A:125:LEU:HD13	1:A:142:LEU:HD23	0.64	1.70	3	1
1:A:142:LEU:HD13	1:A:153:TYR:CE1	0.63	2.28	5	1
1:A:122:HIS:O	1:A:123:ILE:HG23	0.63	1.93	5	1
1:A:194:ILE:HG13	1:A:206:VAL:HG22	0.62	1.69	6	1
1:A:170:ALA:HB1	1:A:181:HIS:CE1	0.62	2.30	5	1
1:A:24:PHE:CE1	1:A:26:LEU:HD13	0.62	2.29	6	1
1:A:143:VAL:O	1:A:144:LEU:HD23	0.62	1.94	9	1
1:A:91:LEU:HD12	1:A:93:ARG:O	0.62	1.95	2	1
1:A:123:ILE:HG23	1:A:144:LEU:HB3	0.62	1.69	2	2
1:A:129:MET:HB3	1:A:138:ILE:HG22	0.61	1.69	1	1
1:A:208:LEU:HD13	1:A:219:PHE:CD2	0.61	2.31	2	1
1:A:27:ILE:HG22	1:A:29:LEU:HD21	0.61	1.70	5	1
1:A:244:GLY:O	1:A:245:LEU:HD22	0.61	1.94	2	1
1:A:262:LEU:CB	1:A:275:LEU:HD13	0.60	2.26	4	1
1:A:72:THR:HG23	1:A:84:GLU:CB	0.60	2.26	2	1
1:A:242:LEU:CD2	1:A:262:LEU:HD21	0.60	2.25	4	1
1:A:209:ALA:HB3	1:A:218:ARG:CB	0.60	2.25	4	2
1:A:209:ALA:HB3	1:A:218:ARG:HB3	0.60	1.72	7	5
1:A:209:ALA:HB3	1:A:218:ARG:HB2	0.60	1.73	6	3
1:A:248:THR:CG2	1:A:258:THR:HG22	0.60	2.25	1	1
1:A:57:SER:O	1:A:58:LEU:HB2	0.60	1.95	2	1
1:A:125:LEU:C	1:A:125:LEU:HD22	0.60	2.16	9	1
1:A:206:VAL:HG12	1:A:221:ILE:CG2	0.60	2.23	10	1
1:A:150:LEU:HD13	1:A:181:HIS:CB	0.60	2.26	2	1
1:A:231:ALA:HB2	1:A:249:GLN:OE1	0.59	1.96	5	1
1:A:116:THR:OG1	1:A:127:ALA:HB3	0.59	1.97	5	1
1:A:259:LEU:HD13	1:A:277:LEU:HD12	0.59	1.75	8	1
1:A:257:LEU:HD21	1:A:259:LEU:CD1	0.59	2.27	4	1
1:A:72:THR:HG23	1:A:84:GLU:HB2	0.59	1.75	7	1
1:A:39:LEU:HD12	1:A:41:PHE:CE2	0.59	2.33	5	1
1:A:69:LEU:HD12	1:A:87:VAL:HG22	0.58	1.74	4	1
1:A:217:THR:HG23	1:A:240:SER:CB	0.58	2.28	8	1
1:A:125:LEU:HD13	1:A:142:LEU:HD12	0.58	1.74	8	1
1:A:24:PHE:CE1	1:A:242:LEU:HD13	0.58	2.34	5	1
1:A:42:THR:HG23	1:A:59:GLU:HB2	0.58	1.76	4	1
1:A:212:ALA:O	1:A:213:GLY:C	0.58	2.42	6	2
1:A:27:ILE:HG22	1:A:277:LEU:HB3	0.58	1.76	3	1
1:A:28:LYS:O	1:A:29:LEU:HD22	0.57	1.99	9	1
1:A:75:TRP:O	1:A:76:ASN:CB	0.57	2.52	4	4
1:A:39:LEU:HD22	1:A:62:TYR:CE1	0.57	2.33	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:HG23	1:A:277:LEU:CB	0.57	2.29	5	1
1:A:242:LEU:CD1	1:A:262:LEU:HD11	0.57	2.29	10	1
1:A:27:ILE:HG23	1:A:277:LEU:HB2	0.57	1.76	5	1
1:A:39:LEU:HD13	1:A:62:TYR:CZ	0.57	2.34	8	1
1:A:63:ARG:HB3	1:A:70:THR:HG23	0.57	1.75	1	1
1:A:69:LEU:CD1	1:A:87:VAL:HG22	0.57	2.30	4	2
1:A:180:LEU:HA	1:A:194:ILE:HG22	0.57	1.76	1	1
1:A:31:LEU:HD23	1:A:281:PHE:CZ	0.57	2.35	3	1
1:A:118:TYR:CE2	1:A:125:LEU:HD11	0.56	2.35	10	1
1:A:118:TYR:CZ	1:A:125:LEU:HD21	0.56	2.35	10	1
1:A:123:ILE:HG23	1:A:144:LEU:CB	0.56	2.30	2	2
1:A:80:THR:O	1:A:81:LEU:HD22	0.56	2.00	6	1
1:A:100:ASP:O	1:A:112:ALA:HB1	0.56	2.00	2	1
1:A:27:ILE:CD1	1:A:47:ALA:HB3	0.56	2.31	3	1
1:A:73:VAL:HG22	1:A:83:THR:HG23	0.56	1.77	7	1
1:A:194:ILE:CG1	1:A:206:VAL:HG22	0.55	2.31	6	1
1:A:202:LEU:N	1:A:202:LEU:HD13	0.55	2.15	5	1
1:A:150:LEU:HD12	1:A:181:HIS:NE2	0.55	2.16	6	1
1:A:202:LEU:HD23	1:A:203:GLU:N	0.55	2.17	1	2
1:A:125:LEU:CD1	1:A:142:LEU:HD23	0.55	2.32	3	1
1:A:84:GLU:CB	1:A:100:ASP:HA	0.55	2.32	10	1
1:A:98:THR:HG23	1:A:115:LYS:HB2	0.55	1.78	4	1
1:A:150:LEU:HD13	1:A:181:HIS:HB3	0.54	1.79	2	1
1:A:86:THR:HG23	1:A:98:THR:CG2	0.54	2.30	10	1
1:A:56:GLY:O	1:A:76:ASN:HB3	0.54	2.02	1	3
1:A:262:LEU:HB2	1:A:275:LEU:HD13	0.54	1.79	4	1
1:A:259:LEU:HD23	1:A:260:SER:N	0.54	2.18	1	2
1:A:69:LEU:HD11	1:A:87:VAL:CG1	0.54	2.31	5	1
1:A:69:LEU:HD22	1:A:87:VAL:CG1	0.54	2.32	9	1
1:A:73:VAL:HG22	1:A:83:THR:CG2	0.53	2.33	7	1
1:A:27:ILE:HD11	1:A:47:ALA:HB3	0.53	1.80	3	1
1:A:118:TYR:CE2	1:A:125:LEU:HD21	0.53	2.39	10	1
1:A:248:THR:HG22	1:A:258:THR:HG23	0.53	1.78	3	1
1:A:43:SER:HA	1:A:58:LEU:HD13	0.53	1.78	10	1
1:A:42:THR:O	1:A:58:LEU:HB3	0.53	2.04	2	1
1:A:30:ASP:O	1:A:281:PHE:N	0.53	2.42	5	2
1:A:244:GLY:C	1:A:245:LEU:HD13	0.53	2.24	7	1
1:A:245:LEU:HD13	1:A:245:LEU:N	0.53	2.19	7	1
1:A:245:LEU:CD2	1:A:261:ALA:HB3	0.53	2.34	7	1
1:A:194:ILE:CG1	1:A:206:VAL:HG23	0.53	2.34	7	1
1:A:211:THR:HG23	1:A:213:GLY:H	0.52	1.64	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:GLU:O	1:A:281:PHE:C	0.52	2.48	4	2
1:A:211:THR:HG22	1:A:217:THR:OG1	0.52	2.04	5	1
1:A:228:ASP:HB2	1:A:231:ALA:HB3	0.52	1.81	9	2
1:A:142:LEU:HD12	1:A:153:TYR:HB2	0.52	1.81	10	1
1:A:123:ILE:HG22	1:A:125:LEU:CD2	0.52	2.35	3	1
1:A:72:THR:HG23	1:A:84:GLU:HB3	0.52	1.82	2	1
1:A:263:LEU:HD23	1:A:273:HIS:ND1	0.52	2.20	2	1
1:A:263:LEU:HD23	1:A:264:ASP:N	0.52	2.20	3	1
1:A:259:LEU:HD12	1:A:277:LEU:CD1	0.51	2.35	3	1
1:A:57:SER:HA	1:A:76:ASN:CB	0.51	2.34	1	3
1:A:211:THR:HB	1:A:217:THR:HG21	0.51	1.82	5	1
1:A:206:VAL:CG1	1:A:221:ILE:HG23	0.51	2.36	7	1
1:A:98:THR:HG23	1:A:115:LYS:CB	0.51	2.36	4	1
1:A:97:LEU:HD23	1:A:116:THR:HB	0.51	1.83	6	1
1:A:75:TRP:O	1:A:76:ASN:HB2	0.51	2.06	1	4
1:A:257:LEU:HD21	1:A:259:LEU:HD12	0.51	1.82	4	1
1:A:231:ALA:HB2	1:A:249:GLN:HG3	0.50	1.83	1	1
1:A:245:LEU:HD13	1:A:263:LEU:HD12	0.50	1.82	5	1
1:A:41:PHE:CD2	1:A:60:THR:HG23	0.50	2.41	5	1
1:A:201:LYS:CB	1:A:202:LEU:HD13	0.50	2.37	5	1
1:A:180:LEU:HD12	1:A:180:LEU:O	0.50	2.07	5	1
1:A:186:ASP:O	1:A:188:THR:HG23	0.50	2.06	8	1
1:A:262:LEU:HD13	1:A:263:LEU:N	0.50	2.22	2	1
1:A:244:GLY:O	1:A:245:LEU:HD12	0.50	2.07	5	1
1:A:248:THR:OG1	1:A:258:THR:HG22	0.49	2.06	2	1
1:A:198:VAL:HG23	1:A:204:THR:HG22	0.49	1.84	3	1
1:A:69:LEU:HD11	1:A:87:VAL:HG13	0.49	1.84	1	1
1:A:256:LYS:O	1:A:257:LEU:HD22	0.49	2.07	7	1
1:A:255:ILE:HD11	1:A:279:LEU:HD11	0.49	1.84	1	1
1:A:80:THR:C	1:A:81:LEU:HD12	0.49	2.28	2	1
1:A:262:LEU:C	1:A:263:LEU:HD12	0.49	2.28	2	1
1:A:123:ILE:CG2	1:A:144:LEU:HD13	0.49	2.37	5	1
1:A:27:ILE:HG22	1:A:29:LEU:CD2	0.49	2.36	5	1
1:A:247:TYR:C	1:A:258:THR:HG23	0.49	2.27	5	1
1:A:189:GLU:HA	1:A:211:THR:HG23	0.49	1.84	9	1
1:A:27:ILE:CG2	1:A:279:LEU:HD23	0.49	2.38	7	1
1:A:123:ILE:CD1	1:A:144:LEU:HD12	0.49	2.37	10	1
1:A:73:VAL:HG21	1:A:75:TRP:CZ3	0.49	2.43	5	1
1:A:42:THR:HG23	1:A:59:GLU:CB	0.48	2.37	4	1
1:A:208:LEU:HD22	1:A:209:ALA:N	0.48	2.23	8	1
1:A:81:LEU:HD12	1:A:81:LEU:O	0.48	2.07	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD13	1:A:62:TYR:CE1	0.48	2.43	8	1
1:A:63:ARG:HG3	1:A:70:THR:HG23	0.48	1.85	7	1
1:A:118:TYR:CD2	1:A:125:LEU:HD11	0.48	2.43	10	1
1:A:257:LEU:HD22	1:A:259:LEU:HD11	0.48	1.84	10	1
1:A:27:ILE:HG23	1:A:277:LEU:HD11	0.48	1.86	10	1
1:A:122:HIS:CB	1:A:123:ILE:HD12	0.48	2.39	2	1
1:A:250:THR:HG22	1:A:256:LYS:CG	0.48	2.39	8	1
1:A:39:LEU:HD12	1:A:61:LYS:O	0.48	2.09	3	1
1:A:125:LEU:HD12	1:A:125:LEU:O	0.47	2.09	10	1
1:A:80:THR:C	1:A:81:LEU:HD22	0.47	2.30	6	1
1:A:69:LEU:HD22	1:A:87:VAL:HA	0.47	1.84	7	1
1:A:123:ILE:CG1	1:A:144:LEU:HD12	0.47	2.38	1	1
1:A:201:LYS:C	1:A:202:LEU:HD13	0.47	2.30	5	1
1:A:188:THR:HG23	1:A:189:GLU:HG2	0.47	1.87	6	1
1:A:39:LEU:HD22	1:A:62:TYR:OH	0.47	2.09	8	1
1:A:26:LEU:O	1:A:26:LEU:HD12	0.47	2.08	10	2
1:A:125:LEU:HD22	1:A:126:GLY:N	0.47	2.24	9	1
1:A:260:SER:HB2	1:A:275:LEU:HD23	0.47	1.85	4	1
1:A:67:TYR:CD1	1:A:69:LEU:HD22	0.47	2.43	8	1
1:A:24:PHE:CD1	1:A:26:LEU:HD22	0.47	2.44	6	1
1:A:63:ARG:CG	1:A:70:THR:HG23	0.46	2.41	7	1
1:A:247:TYR:CE2	1:A:259:LEU:HD13	0.46	2.45	10	1
1:A:122:HIS:CD2	1:A:123:ILE:CG1	0.46	2.98	5	1
1:A:123:ILE:HD11	1:A:125:LEU:HD22	0.46	1.88	7	1
1:A:142:LEU:HD13	1:A:153:TYR:CE2	0.46	2.46	8	1
1:A:43:SER:HA	1:A:58:LEU:CB	0.46	2.40	2	1
1:A:27:ILE:CG2	1:A:29:LEU:HD21	0.46	2.38	5	1
1:A:41:PHE:CG	1:A:60:THR:HG23	0.46	2.45	2	1
1:A:122:HIS:HB2	1:A:123:ILE:HD12	0.46	1.87	2	1
1:A:188:THR:CG2	1:A:212:ALA:HB2	0.46	2.41	2	1
1:A:152:GLY:O	1:A:170:ALA:HB3	0.46	2.11	7	1
1:A:79:ASN:O	1:A:80:THR:HG23	0.46	2.11	8	1
1:A:262:LEU:HB2	1:A:275:LEU:HD12	0.46	1.88	10	1
1:A:94:GLY:O	1:A:95:LEU:HD23	0.45	2.11	5	1
1:A:39:LEU:HD12	1:A:62:TYR:HA	0.45	1.88	1	1
1:A:68:GLY:O	1:A:69:LEU:HD22	0.45	2.11	1	1
1:A:31:LEU:CB	1:A:279:LEU:HD22	0.45	2.42	5	1
1:A:247:TYR:CZ	1:A:259:LEU:HD23	0.45	2.46	8	1
1:A:69:LEU:CD1	1:A:87:VAL:HG12	0.45	2.33	5	1
1:A:131:PHE:HE1	1:A:134:ALA:HB3	0.45	1.72	1	2
1:A:123:ILE:HG22	1:A:144:LEU:HB2	0.45	1.88	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HB3	1:A:279:LEU:HD22	0.45	1.89	5	1
1:A:237:VAL:HG23	1:A:243:ILE:HG12	0.45	1.87	5	1
1:A:152:GLY:CA	1:A:170:ALA:HB3	0.45	2.41	6	1
1:A:244:GLY:C	1:A:245:LEU:HD22	0.44	2.32	2	1
1:A:94:GLY:C	1:A:95:LEU:HD12	0.44	2.33	10	1
1:A:244:GLY:HA2	1:A:262:LEU:HD12	0.44	1.89	4	1
1:A:42:THR:HG22	1:A:59:GLU:HB2	0.44	1.89	5	1
1:A:27:ILE:HG23	1:A:279:LEU:HD23	0.44	1.89	7	1
1:A:209:ALA:O	1:A:218:ARG:N	0.44	2.51	5	3
1:A:123:ILE:HD12	1:A:144:LEU:CD1	0.44	2.41	10	1
1:A:88:GLU:CD	1:A:92:ALA:HB2	0.44	2.33	1	1
1:A:131:PHE:CE1	1:A:134:ALA:HB3	0.44	2.48	1	1
1:A:206:VAL:CG1	1:A:221:ILE:HG22	0.44	2.43	8	1
1:A:44:SER:HB3	1:A:58:LEU:HD23	0.44	1.90	2	1
1:A:84:GLU:C	1:A:85:ILE:HD12	0.44	2.33	4	1
1:A:244:GLY:C	1:A:245:LEU:HD12	0.44	2.33	5	1
1:A:242:LEU:HD22	1:A:262:LEU:HD21	0.44	1.89	10	1
1:A:29:LEU:HB2	1:A:279:LEU:HD12	0.43	1.89	4	1
1:A:57:SER:C	1:A:58:LEU:HD22	0.43	2.34	10	1
1:A:202:LEU:HD12	1:A:225:TYR:CE2	0.43	2.48	1	1
1:A:28:LYS:O	1:A:29:LEU:HD23	0.43	2.14	3	1
1:A:84:GLU:HB2	1:A:101:SER:H	0.43	1.73	10	1
1:A:14:ALA:HB1	1:A:218:ARG:NH1	0.43	2.29	1	1
1:A:42:THR:HG22	1:A:58:LEU:HG	0.42	1.90	2	1
1:A:217:THR:HG23	1:A:240:SER:HB3	0.42	1.91	8	1
1:A:180:LEU:C	1:A:180:LEU:CD2	0.42	2.82	9	1
1:A:57:SER:O	1:A:58:LEU:CB	0.42	2.65	2	1
1:A:61:LYS:HG2	1:A:72:THR:HG23	0.42	1.91	3	1
1:A:259:LEU:CD1	1:A:277:LEU:HD12	0.42	2.44	8	1
1:A:208:LEU:HD12	1:A:208:LEU:O	0.42	2.14	10	1
1:A:205:ALA:HB3	1:A:222:ALA:O	0.42	2.15	5	1
1:A:208:LEU:O	1:A:208:LEU:HD13	0.42	2.13	8	1
1:A:211:THR:O	1:A:217:THR:HG21	0.42	2.14	9	1
1:A:244:GLY:CA	1:A:262:LEU:HD13	0.42	2.44	6	1
1:A:113:LYS:C	1:A:114:ILE:HD12	0.42	2.35	7	1
1:A:277:LEU:HD23	1:A:278:GLY:N	0.42	2.30	4	1
1:A:180:LEU:HD23	1:A:181:HIS:N	0.42	2.30	10	1
1:A:118:TYR:O	1:A:125:LEU:HD23	0.41	2.15	1	1
1:A:208:LEU:HD13	1:A:208:LEU:C	0.41	2.35	8	1
1:A:247:TYR:CE2	1:A:259:LEU:HD23	0.41	2.50	8	1
1:A:68:GLY:C	1:A:69:LEU:HD22	0.41	2.35	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:THR:O	1:A:81:LEU:HD12	0.41	2.15	2	1
1:A:221:ILE:HB	1:A:237:VAL:HG13	0.41	1.92	2	1
1:A:29:LEU:HD22	1:A:279:LEU:HD12	0.41	1.92	3	1
1:A:230:ASP:HB3	1:A:251:LEU:HD22	0.41	1.93	8	1
1:A:250:THR:HG23	1:A:256:LYS:HG3	0.41	1.91	7	1
1:A:95:LEU:HD21	1:A:125:LEU:HD21	0.41	1.93	9	1
1:A:262:LEU:HB3	1:A:275:LEU:HD13	0.41	1.93	4	1
1:A:194:ILE:HG22	1:A:206:VAL:O	0.41	2.15	9	1
1:A:248:THR:HG23	1:A:258:THR:OG1	0.41	2.15	5	1
1:A:186:ASP:HB3	1:A:188:THR:HG22	0.41	1.93	6	1
1:A:217:THR:HG23	1:A:240:SER:HB2	0.41	1.91	8	1
1:A:84:GLU:HB2	1:A:100:ASP:HA	0.41	1.93	10	1
1:A:205:ALA:O	1:A:206:VAL:HG13	0.41	2.15	7	1
1:A:208:LEU:HD23	1:A:219:PHE:CD1	0.41	2.51	8	1
1:A:75:TRP:HB2	1:A:81:LEU:HD13	0.41	1.93	2	1
1:A:60:THR:O	1:A:73:VAL:HG12	0.41	2.16	6	1
1:A:210:TRP:O	1:A:211:THR:HG23	0.41	2.16	9	1
1:A:242:LEU:HD13	1:A:262:LEU:CD1	0.41	2.40	10	1
1:A:208:LEU:HD12	1:A:209:ALA:N	0.40	2.31	2	1
1:A:110:LYS:C	1:A:133:ILE:HD11	0.40	2.37	7	1
1:A:125:LEU:N	1:A:125:LEU:CD1	0.40	2.85	9	1
1:A:237:VAL:HG23	1:A:242:LEU:O	0.40	2.16	3	1
1:A:69:LEU:HD21	1:A:71:PHE:CE2	0.40	2.52	4	1
1:A:256:LYS:C	1:A:257:LEU:HD22	0.40	2.37	7	1
1:A:138:ILE:O	1:A:138:ILE:HD12	0.40	2.16	10	1
1:A:123:ILE:HG13	1:A:144:LEU:HD12	0.40	1.94	1	1
1:A:206:VAL:HG13	1:A:221:ILE:HG22	0.40	1.93	8	1
1:A:63:ARG:HA	1:A:70:THR:HG23	0.40	1.92	9	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	228/291 (78%)	191±4 (84±2%)	32±4 (14±2%)	5±2 (2±1%)	9	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2280/2910 (78%)	1913 (84%)	315 (14%)	52 (2%)	9 48

All 31 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	76	ASN	5
1	A	213	GLY	5
1	A	133	ILE	4
1	A	68	GLY	3
1	A	134	ALA	3
1	A	218	ARG	3
1	A	37	ASN	2
1	A	89	ASP	2
1	A	178	PHE	2
1	A	81	LEU	2
1	A	57	SER	1
1	A	58	LEU	1
1	A	135	GLY	1
1	A	88	GLU	1
1	A	93	ARG	1
1	A	77	THR	1
1	A	147	GLU	1
1	A	175	THR	1
1	A	275	LEU	1
1	A	25	GLY	1
1	A	65	THR	1
1	A	64	TRP	1
1	A	211	THR	1
1	A	217	THR	1
1	A	38	GLY	1
1	A	131	PHE	1
1	A	132	ASP	1
1	A	102	SER	1
1	A	78	ASP	1
1	A	91	LEU	1
1	A	84	GLU	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	186/237 (78%)	162±6 (87±3%)	24±6 (13±3%)	7	48
All	All	1860/2370 (78%)	1618 (87%)	242 (13%)	7	48

All 117 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	101	SER	7
1	A	70	THR	6
1	A	119	LYS	6
1	A	81	LEU	5
1	A	211	THR	5
1	A	214	ASN	5
1	A	33	THR	4
1	A	46	SER	4
1	A	76	ASN	4
1	A	175	THR	4
1	A	197	LYS	4
1	A	208	LEU	4
1	A	217	THR	4
1	A	228	ASP	4
1	A	236	LYS	4
1	A	142	LEU	4
1	A	182	THR	4
1	A	218	ARG	4
1	A	80	THR	4
1	A	42	THR	3
1	A	131	PHE	3
1	A	245	LEU	3
1	A	58	LEU	3
1	A	72	THR	3
1	A	124	ASN	3
1	A	100	ASP	3
1	A	180	LEU	3
1	A	260	SER	3
1	A	15	ARG	3
1	A	259	LEU	3
1	A	113	LYS	3
1	A	26	LEU	2
1	A	31	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	55	THR	2
1	A	200	LYS	2
1	A	232	SER	2
1	A	75	TRP	2
1	A	168	ASN	2
1	A	275	LEU	2
1	A	44	SER	2
1	A	61	LYS	2
1	A	125	LEU	2
1	A	238	ASN	2
1	A	274	LYS	2
1	A	28	LYS	2
1	A	29	LEU	2
1	A	30	ASP	2
1	A	64	TRP	2
1	A	115	LYS	2
1	A	138	ILE	2
1	A	216	ASN	2
1	A	234	SER	2
1	A	43	SER	2
1	A	65	THR	2
1	A	86	THR	2
1	A	110	LYS	2
1	A	173	TYR	2
1	A	202	LEU	2
1	A	60	THR	2
1	A	83	THR	2
1	A	240	SER	2
1	A	102	SER	2
1	A	146	TYR	2
1	A	174	LYS	2
1	A	155	MET	2
1	A	48	ASN	1
1	A	74	LYS	1
1	A	130	ASP	1
1	A	185	ASN	1
1	A	226	GLN	1
1	A	32	LYS	1
1	A	78	ASP	1
1	A	91	LEU	1
1	A	224	LYS	1
1	A	262	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	179	GLN	1
1	A	225	TYR	1
1	A	257	LEU	1
1	A	77	THR	1
1	A	79	ASN	1
1	A	95	LEU	1
1	A	129	MET	1
1	A	132	ASP	1
1	A	144	LEU	1
1	A	280	GLU	1
1	A	39	LEU	1
1	A	84	GLU	1
1	A	93	ARG	1
1	A	97	LEU	1
1	A	123	ILE	1
1	A	210	TRP	1
1	A	281	PHE	1
1	A	62	TYR	1
1	A	67	TYR	1
1	A	98	THR	1
1	A	178	PHE	1
1	A	183	ASN	1
1	A	227	ILE	1
1	A	277	LEU	1
1	A	204	THR	1
1	A	206	VAL	1
1	A	247	TYR	1
1	A	255	ILE	1
1	A	85	ILE	1
1	A	96	LYS	1
1	A	251	LEU	1
1	A	59	GLU	1
1	A	69	LEU	1
1	A	137	SER	1
1	A	194	ILE	1
1	A	201	LYS	1
1	A	241	SER	1
1	A	37	ASN	1
1	A	57	SER	1
1	A	71	PHE	1
1	A	186	ASP	1
1	A	193	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

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 31% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 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	1056
Number of shifts mapped to atoms	1056
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	198	$0.64 \pm 0.06$	Should be applied
$^{13}\text{C}_\beta$	159	$-0.39 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	174	$0.85 \pm 0.11$	Should be applied
$^{15}\text{N}$	192	$-0.20 \pm 0.48$	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 35%, i.e. 945 atoms were assigned a chemical shift out of a possible 2714. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	798/1141 (70%)	282/456 (62%)	340/458 (74%)	176/227 (78%)
Sidechain	147/1333 (11%)	0/771 (0%)	147/503 (29%)	0/59 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/240 (0%)	0/127 (0%)	0/106 (0%)	0/7 (0%)
Overall	945/2714 (35%)	282/1354 (21%)	487/1067 (46%)	176/293 (60%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 31%, i.e. 1035 atoms were assigned a chemical shift out of a possible 3328. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	876/1403 (62%)	312/560 (56%)	372/566 (66%)	192/277 (69%)
Sidechain	159/1642 (10%)	0/954 (0%)	159/615 (26%)	0/73 (0%)
Aromatic	0/283 (0%)	0/150 (0%)	0/126 (0%)	0/7 (0%)
Overall	1035/3328 (31%)	312/1664 (19%)	531/1307 (41%)	192/357 (54%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

#### 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:

