



Full wwPDB NMR Structure Validation Report ⓘ

May 31, 2020 – 11:10 am BST

PDB ID : 6KR8
Title : Structure of the beta2 adrenergic receptor in the full agonist bound state
Authors : Imai, S.; Shimada, I.
Deposited on : 2019-08-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

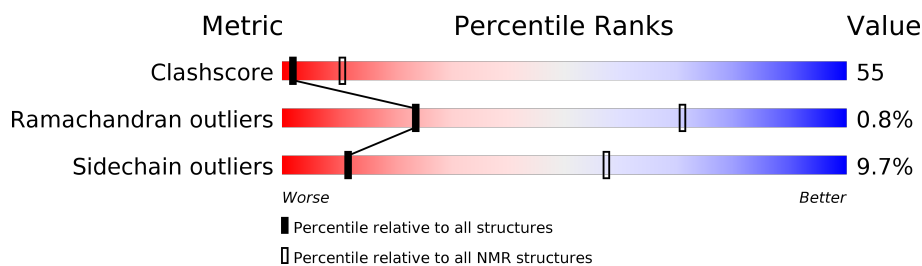
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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 ≥ 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	336	

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:30-A:55, A:63-A:133, A:141-A:144, A:150-A:237, A:273-A:341 (258)	0.07	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.

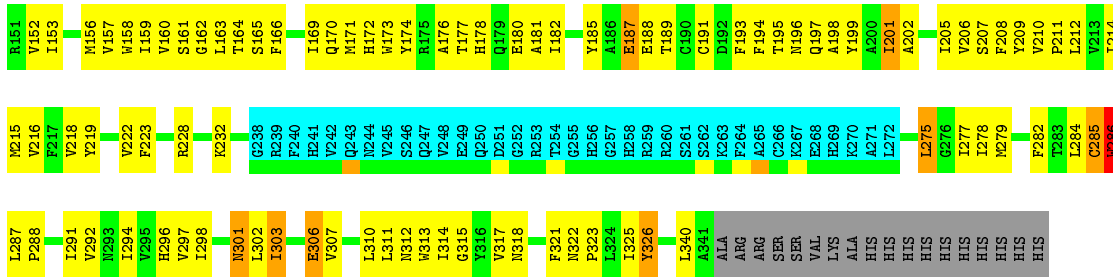
Cluster number	Models
1	2, 4, 5, 7, 8, 9
2	1, 3, 10
Single-model clusters	6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5052 atoms, of which 2544 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called beta 2 adrenergic receptor.

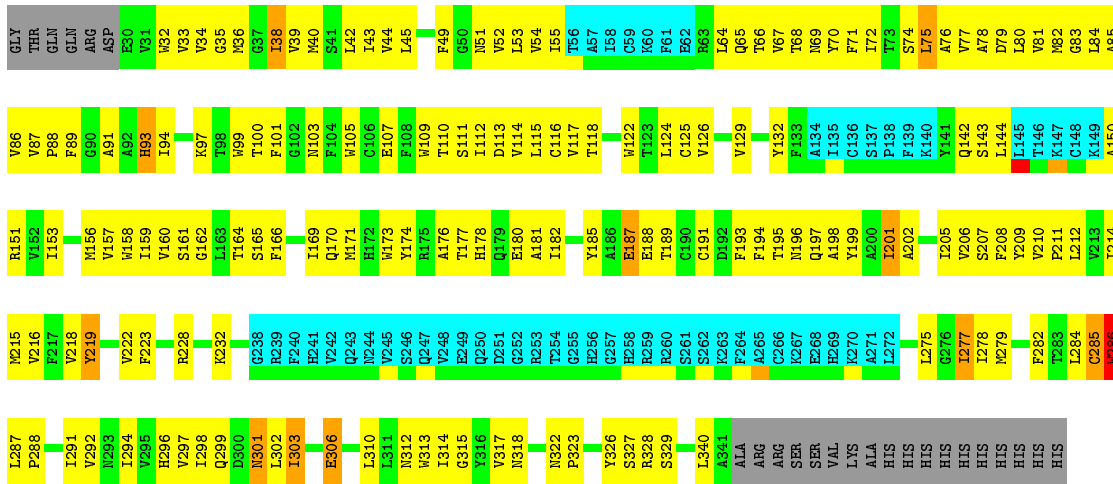
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	312	5052	1651	2544	413	425	19	0



4.2.2 Score per residue for model 2

- Molecule 1: beta 2 adrenergic receptor

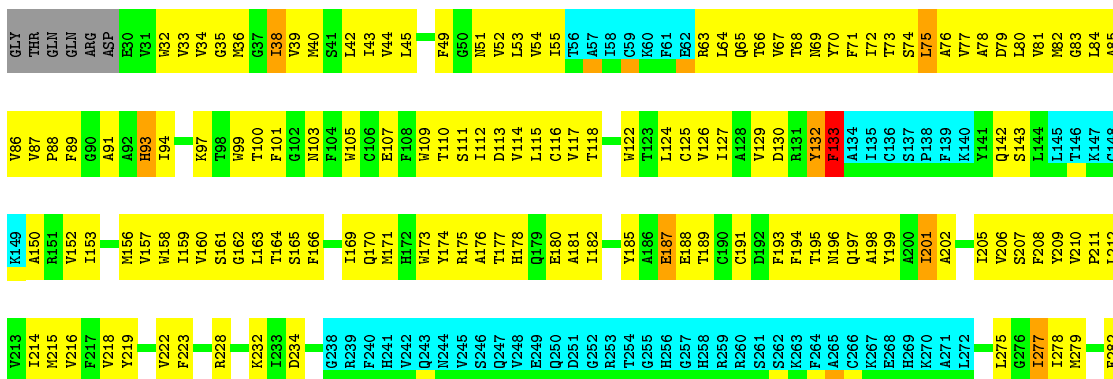
Chain A: 29% 45% 16% 7%



4.2.3 Score per residue for model 3

- Molecule 1: beta 2 adrenergic receptor

Chain A: 26% 46% 16% 7%



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
X-PLOR NIH	structure calculation	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	38
Number of shifts mapped to atoms	19
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	19
Assignment completeness (well-defined parts)	1%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

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 i

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	2082	2114	2106	232±6
All	All	20820	21140	21060	2323

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 55.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:CYS:O	1:A:286:TRP:CG	1.07	2.08	7	10
1:A:285:CYS:O	1:A:286:TRP:CD1	0.98	2.17	7	8
1:A:176:ALA:HB3	1:A:194:PHE:HE2	0.90	1.25	1	10
1:A:285:CYS:HB3	1:A:314:ILE:O	0.90	1.66	5	10
1:A:36:MET:HG2	1:A:40:MET:HE2	0.89	1.42	1	10
1:A:285:CYS:CB	1:A:314:ILE:O	0.88	2.21	7	10
1:A:275:LEU:HD23	1:A:275:LEU:O	0.87	1.69	9	2
1:A:117:VAL:HG23	1:A:286:TRP:CZ2	0.84	2.07	10	2
1:A:287:LEU:HD13	1:A:291:ILE:HD13	0.84	1.50	1	10
1:A:117:VAL:HG23	1:A:286:TRP:CH2	0.83	2.07	10	10
1:A:176:ALA:HB3	1:A:194:PHE:CE2	0.82	2.09	1	10
1:A:285:CYS:O	1:A:286:TRP:CB	0.82	2.27	5	10
1:A:114:VAL:HG23	1:A:165:SER:HB3	0.81	1.51	1	10
1:A:275:LEU:HD23	1:A:276:GLY:N	0.81	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:314:ILE:O	1:A:317:VAL:HG12	0.81	1.75	1	10
1:A:219:TYR:HB2	1:A:275:LEU:HG	0.80	1.52	6	1
1:A:278:ILE:HG22	1:A:279:MET:N	0.79	1.90	4	10
1:A:169:ILE:HA	1:A:174:TYR:CE2	0.79	2.13	1	10
1:A:285:CYS:HB2	1:A:315:GLY:HA2	0.78	1.55	5	10
1:A:311:LEU:O	1:A:314:ILE:HG22	0.78	1.77	5	2
1:A:219:TYR:CD1	1:A:275:LEU:HD11	0.78	2.14	2	2
1:A:310:LEU:O	1:A:314:ILE:HG12	0.78	1.79	3	3
1:A:310:LEU:O	1:A:314:ILE:HG13	0.78	1.79	1	2
1:A:286:TRP:CE3	1:A:286:TRP:HA	0.77	2.14	6	4
1:A:49:PHE:CE2	1:A:53:LEU:HD11	0.76	2.15	1	10
1:A:54:VAL:O	1:A:55:ILE:C	0.75	2.22	5	1
1:A:286:TRP:HA	1:A:286:TRP:CE3	0.75	2.15	10	6
1:A:210:VAL:HB	1:A:211:PRO:HD3	0.74	1.60	1	10
1:A:117:VAL:CG2	1:A:286:TRP:CH2	0.74	2.70	10	2
1:A:275:LEU:HD23	1:A:275:LEU:C	0.74	2.03	9	2
1:A:228:ARG:HB3	1:A:232:LYS:HE2	0.73	1.56	1	10
1:A:122:TRP:CD1	1:A:157:VAL:HG13	0.73	2.19	1	10
1:A:285:CYS:O	1:A:286:TRP:HB2	0.73	1.82	10	10
1:A:122:TRP:CD1	1:A:157:VAL:HG22	0.73	2.18	1	10
1:A:219:TYR:O	1:A:222:VAL:HG12	0.73	1.84	1	10
1:A:121:ILE:HD11	1:A:286:TRP:NE1	0.73	1.97	10	2
1:A:109:TRP:O	1:A:112:ILE:HG22	0.72	1.85	1	10
1:A:121:ILE:HD11	1:A:286:TRP:CD1	0.72	2.20	10	2
1:A:114:VAL:CG2	1:A:165:SER:HB3	0.71	2.15	1	10
1:A:82:MET:HB2	1:A:116:CYS:SG	0.71	2.26	1	10
1:A:83:GLY:HA2	1:A:87:VAL:HG12	0.71	1.63	1	10
1:A:67:VAL:HA	1:A:70:TYR:CD1	0.70	2.20	9	10
1:A:212:LEU:O	1:A:216:VAL:HG23	0.70	1.86	1	10
1:A:304:ARG:O	1:A:307:VAL:HG22	0.70	1.87	10	2
1:A:38:ILE:HD13	1:A:42:LEU:HD13	0.70	1.60	1	10
1:A:219:TYR:C	1:A:219:TYR:CD1	0.69	2.65	9	3
1:A:212:LEU:HD13	1:A:282:PHE:CD2	0.69	2.21	3	8
1:A:51:ASN:O	1:A:54:VAL:HG12	0.69	1.88	1	10
1:A:107:GLU:O	1:A:110:THR:HG22	0.69	1.87	1	10
1:A:156:MET:O	1:A:159:ILE:HG22	0.68	1.88	1	10
1:A:171:MET:HG2	1:A:173:TRP:NE1	0.68	2.02	1	10
1:A:287:LEU:O	1:A:291:ILE:HD13	0.68	1.87	1	10
1:A:36:MET:CE	1:A:94:ILE:HD12	0.68	2.18	1	10
1:A:75:LEU:HD21	1:A:124:LEU:CD2	0.68	2.19	1	10
1:A:99:TRP:O	1:A:189:THR:HG23	0.68	1.89	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:286:TRP:HE3	1:A:286:TRP:HA	0.67	1.48	6	2
1:A:284:LEU:O	1:A:314:ILE:CG2	0.67	2.42	10	8
1:A:285:CYS:HB3	1:A:314:ILE:C	0.66	2.11	1	2
1:A:197:GLN:HG2	1:A:297:VAL:CG2	0.66	2.20	1	10
1:A:178:HIS:CD2	1:A:180:GLU:H	0.65	2.08	1	10
1:A:74:SER:O	1:A:77:VAL:HG12	0.65	1.91	1	10
1:A:285:CYS:HB2	1:A:314:ILE:O	0.65	1.91	7	8
1:A:286:TRP:CZ2	1:A:315:GLY:O	0.65	2.49	7	2
1:A:40:MET:O	1:A:44:VAL:HG23	0.65	1.92	1	10
1:A:285:CYS:HB3	1:A:314:ILE:HG22	0.64	1.67	7	7
1:A:286:TRP:HA	1:A:286:TRP:HE3	0.64	1.50	10	5
1:A:40:MET:SD	1:A:91:ALA:HB1	0.64	2.32	1	10
1:A:153:ILE:O	1:A:157:VAL:HG23	0.64	1.93	1	10
1:A:71:PHE:CZ	1:A:150:ALA:HB1	0.64	2.27	2	4
1:A:219:TYR:HB2	1:A:275:LEU:CG	0.63	2.22	6	1
1:A:169:ILE:HA	1:A:174:TYR:CD2	0.63	2.29	1	10
1:A:288:PRO:O	1:A:292:VAL:HG23	0.63	1.93	1	10
1:A:115:LEU:HB2	1:A:166:PHE:CE1	0.63	2.28	1	10
1:A:78:ALA:O	1:A:81:VAL:HG12	0.63	1.93	1	10
1:A:36:MET:HG2	1:A:40:MET:CE	0.62	2.22	1	10
1:A:219:TYR:CD1	1:A:219:TYR:C	0.62	2.72	2	2
1:A:171:MET:HG2	1:A:173:TRP:CE2	0.62	2.30	1	10
1:A:197:GLN:HG2	1:A:297:VAL:HG21	0.62	1.70	1	10
1:A:80:LEU:HD23	1:A:80:LEU:O	0.61	1.95	1	5
1:A:80:LEU:O	1:A:80:LEU:HD23	0.61	1.95	3	5
1:A:314:ILE:CG2	1:A:315:GLY:N	0.61	2.63	9	2
1:A:176:ALA:CB	1:A:194:PHE:HE2	0.61	2.07	1	10
1:A:219:TYR:CD1	1:A:275:LEU:HD12	0.61	2.30	7	1
1:A:187:GLU:OE1	1:A:189:THR:HB	0.61	1.96	1	10
1:A:205:ILE:HA	1:A:209:TYR:HD1	0.61	1.53	1	10
1:A:165:SER:O	1:A:169:ILE:HG12	0.60	1.95	1	10
1:A:161:SER:O	1:A:164:THR:HG22	0.60	1.96	1	10
1:A:36:MET:O	1:A:40:MET:HG3	0.60	1.96	1	10
1:A:228:ARG:O	1:A:232:LYS:HG3	0.60	1.96	1	10
1:A:86:VAL:HG22	1:A:112:ILE:HG23	0.60	1.74	1	10
1:A:275:LEU:CD2	1:A:279:MET:SD	0.60	2.89	9	1
1:A:277:ILE:HG21	1:A:326:TYR:CD1	0.59	2.32	3	8
1:A:306:GLU:O	1:A:310:LEU:HD13	0.59	1.98	1	10
1:A:285:CYS:HA	1:A:314:ILE:HG23	0.59	1.74	9	2
1:A:205:ILE:HA	1:A:209:TYR:CD1	0.59	2.33	1	10
1:A:55:ILE:HG23	1:A:55:ILE:O	0.59	1.95	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:TYR:O	1:A:133:PHE:C	0.58	2.39	3	3
1:A:115:LEU:HD11	1:A:158:TRP:CZ3	0.58	2.33	1	10
1:A:278:ILE:CG2	1:A:279:MET:N	0.58	2.61	10	10
1:A:321:PHE:O	1:A:325:ILE:HG12	0.58	1.98	6	7
1:A:55:ILE:HG21	1:A:73:THR:HG23	0.58	1.74	7	2
1:A:287:LEU:HD13	1:A:291:ILE:CD1	0.57	2.28	1	10
1:A:36:MET:CG	1:A:40:MET:HE2	0.57	2.23	1	10
1:A:87:VAL:CG1	1:A:88:PRO:HD3	0.57	2.29	1	10
1:A:286:TRP:CZ3	1:A:315:GLY:HA3	0.57	2.33	6	2
1:A:215:MET:SD	1:A:278:ILE:CG2	0.57	2.93	7	4
1:A:275:LEU:C	1:A:275:LEU:CD2	0.56	2.72	9	1
1:A:103:ASN:HB2	1:A:188:GLU:HA	0.56	1.77	1	10
1:A:115:LEU:O	1:A:115:LEU:HD13	0.56	2.00	1	8
1:A:115:LEU:HD13	1:A:115:LEU:O	0.56	2.00	2	2
1:A:219:TYR:HB3	1:A:275:LEU:HD12	0.56	1.78	1	2
1:A:286:TRP:CE3	1:A:315:GLY:HA3	0.56	2.36	6	2
1:A:121:ILE:CD1	1:A:286:TRP:CD1	0.56	2.88	10	2
1:A:45:LEU:HD23	1:A:45:LEU:O	0.56	2.01	1	8
1:A:45:LEU:O	1:A:45:LEU:HD23	0.56	2.01	3	2
1:A:169:ILE:HA	1:A:174:TYR:HE2	0.56	1.59	1	10
1:A:285:CYS:HB2	1:A:315:GLY:CA	0.56	2.31	5	9
1:A:114:VAL:HG23	1:A:165:SER:CB	0.55	2.28	1	10
1:A:157:VAL:O	1:A:160:VAL:HG12	0.55	2.00	1	10
1:A:219:TYR:CB	1:A:275:LEU:HD13	0.55	2.31	5	2
1:A:211:PRO:O	1:A:215:MET:HG2	0.55	2.01	1	10
1:A:33:VAL:HG13	1:A:34:VAL:N	0.55	2.17	1	10
1:A:219:TYR:CG	1:A:275:LEU:HD23	0.55	2.37	3	1
1:A:67:VAL:HG13	1:A:68:THR:N	0.55	2.16	4	3
1:A:206:VAL:HG23	1:A:207:SER:N	0.55	2.16	1	10
1:A:133:PHE:CE1	1:A:141:TYR:CG	0.55	2.94	6	1
1:A:115:LEU:HD23	1:A:162:GLY:HA2	0.55	1.76	1	10
1:A:198:ALA:HA	1:A:201:ILE:CD1	0.55	2.31	1	10
1:A:89:PHE:CD2	1:A:101:PHE:CZ	0.55	2.95	1	10
1:A:277:ILE:HG22	1:A:278:ILE:N	0.55	2.17	2	1
1:A:208:PHE:CE1	1:A:282:PHE:CD2	0.55	2.94	3	1
1:A:38:ILE:O	1:A:42:LEU:HD13	0.54	2.01	1	10
1:A:89:PHE:CE2	1:A:101:PHE:CE2	0.54	2.95	1	10
1:A:307:VAL:CG2	1:A:308:TYR:N	0.54	2.70	4	2
1:A:303:ILE:HD13	1:A:303:ILE:N	0.54	2.17	1	8
1:A:303:ILE:N	1:A:303:ILE:HD13	0.54	2.17	5	2
1:A:38:ILE:HD13	1:A:42:LEU:CD1	0.54	2.33	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:ILE:CG2	1:A:278:ILE:N	0.54	2.70	2	1
1:A:67:VAL:HG23	1:A:68:THR:N	0.54	2.16	3	1
1:A:288:PRO:HB2	1:A:311:LEU:HD22	0.54	1.78	10	1
1:A:294:ILE:O	1:A:297:VAL:HG12	0.54	2.02	1	10
1:A:178:HIS:HD2	1:A:180:GLU:H	0.53	1.46	1	10
1:A:287:LEU:HD13	1:A:287:LEU:O	0.53	2.03	1	7
1:A:287:LEU:O	1:A:287:LEU:HD13	0.53	2.03	10	3
1:A:117:VAL:CG2	1:A:286:TRP:CZ2	0.53	2.90	10	1
1:A:115:LEU:HB2	1:A:166:PHE:HE1	0.53	1.63	1	10
1:A:35:GLY:O	1:A:38:ILE:HG22	0.53	2.03	1	10
1:A:97:LYS:HG3	1:A:97:LYS:O	0.53	2.04	1	6
1:A:97:LYS:O	1:A:97:LYS:HG3	0.53	2.04	2	4
1:A:281:THR:O	1:A:285:CYS:O	0.53	2.27	5	3
1:A:285:CYS:CB	1:A:314:ILE:HG22	0.53	2.34	7	1
1:A:205:ILE:HG13	1:A:206:VAL:N	0.52	2.20	1	10
1:A:303:ILE:HD13	1:A:303:ILE:H	0.52	1.63	1	6
1:A:303:ILE:H	1:A:303:ILE:HD13	0.52	1.63	2	4
1:A:89:PHE:HD2	1:A:101:PHE:CZ	0.52	2.22	1	10
1:A:208:PHE:CE1	1:A:282:PHE:CE2	0.52	2.97	3	1
1:A:114:VAL:O	1:A:117:VAL:HG12	0.52	2.05	1	10
1:A:288:PRO:HG2	1:A:311:LEU:HD11	0.52	1.79	7	4
1:A:277:ILE:HD11	1:A:325:ILE:HB	0.52	1.82	3	1
1:A:287:LEU:HB3	1:A:288:PRO:CD	0.52	2.34	1	10
1:A:51:ASN:OD1	1:A:79:ASP:HB2	0.52	2.04	1	10
1:A:322:ASN:O	1:A:326:TYR:N	0.52	2.42	5	8
1:A:125:CYS:HB3	1:A:211:PRO:HB3	0.52	1.81	1	10
1:A:289:PHE:HB2	1:A:311:LEU:HD12	0.52	1.82	7	4
1:A:178:HIS:O	1:A:182:ILE:HG13	0.52	2.04	1	10
1:A:115:LEU:CD1	1:A:158:TRP:HZ3	0.52	2.18	1	10
1:A:169:ILE:HD13	1:A:174:TYR:CD2	0.52	2.39	1	10
1:A:196:ASN:HD21	1:A:199:TYR:HB2	0.51	1.65	1	10
1:A:177:THR:HG23	1:A:177:THR:O	0.51	2.05	1	3
1:A:215:MET:HE1	1:A:282:PHE:CE1	0.51	2.40	1	6
1:A:177:THR:O	1:A:177:THR:HG23	0.51	2.05	2	7
1:A:277:ILE:HD13	1:A:277:ILE:N	0.51	2.19	10	1
1:A:75:LEU:CD2	1:A:124:LEU:HD23	0.51	2.34	1	10
1:A:36:MET:SD	1:A:94:ILE:HD12	0.51	2.45	1	10
1:A:67:VAL:HA	1:A:70:TYR:CE1	0.51	2.39	9	10
1:A:307:VAL:HG23	1:A:308:TYR:N	0.51	2.20	10	2
1:A:75:LEU:HD21	1:A:124:LEU:HD21	0.51	1.82	1	10
1:A:166:PHE:O	1:A:170:GLN:HG2	0.51	2.05	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:ARG:CB	1:A:232:LYS:HE2	0.51	2.34	1	10
1:A:84:LEU:O	1:A:88:PRO:HG2	0.51	2.05	1	10
1:A:212:LEU:HD13	1:A:282:PHE:HD2	0.51	1.66	10	1
1:A:284:LEU:O	1:A:314:ILE:HG22	0.50	2.04	10	5
1:A:133:PHE:C	1:A:133:PHE:CD1	0.50	2.79	6	1
1:A:202:ALA:O	1:A:206:VAL:HG22	0.50	2.06	1	10
1:A:115:LEU:CB	1:A:166:PHE:HE1	0.50	2.19	1	10
1:A:193:PHE:CZ	1:A:195:THR:CG2	0.50	2.94	1	10
1:A:296:HIS:HA	1:A:303:ILE:HD11	0.50	1.83	1	10
1:A:286:TRP:HE1	1:A:318:ASN:CG	0.50	2.10	7	2
1:A:228:ARG:HB3	1:A:232:LYS:CE	0.50	2.32	1	10
1:A:215:MET:CE	1:A:282:PHE:CZ	0.50	2.94	10	1
1:A:285:CYS:C	1:A:286:TRP:CG	0.49	2.84	7	3
1:A:201:ILE:H	1:A:201:ILE:HD13	0.49	1.67	1	6
1:A:201:ILE:HD13	1:A:201:ILE:H	0.49	1.67	2	4
1:A:38:ILE:C	1:A:38:ILE:HD13	0.49	2.27	1	9
1:A:133:PHE:CE1	1:A:141:TYR:CD1	0.49	3.01	6	1
1:A:38:ILE:HD13	1:A:38:ILE:C	0.49	2.27	10	1
1:A:39:VAL:HG12	1:A:43:ILE:HD13	0.49	1.84	1	10
1:A:275:LEU:O	1:A:275:LEU:HD22	0.49	2.07	3	1
1:A:198:ALA:HA	1:A:201:ILE:HD11	0.49	1.84	1	10
1:A:133:PHE:O	1:A:133:PHE:CG	0.49	2.62	6	1
1:A:299:GLN:HG3	1:A:302:LEU:HD12	0.49	1.84	6	1
1:A:210:VAL:O	1:A:214:ILE:HD13	0.48	2.08	1	10
1:A:49:PHE:CE2	1:A:53:LEU:CD1	0.48	2.94	1	10
1:A:127:ILE:HG21	1:A:326:TYR:OH	0.48	2.08	3	1
1:A:169:ILE:CA	1:A:174:TYR:HE2	0.48	2.21	1	10
1:A:314:ILE:HG22	1:A:315:GLY:N	0.48	2.23	9	2
1:A:130:ASP:O	1:A:133:PHE:HB2	0.48	2.07	3	1
1:A:75:LEU:HD21	1:A:124:LEU:HD23	0.48	1.85	1	10
1:A:93:HIS:HB2	1:A:99:TRP:CZ3	0.48	2.44	1	10
1:A:54:VAL:HG13	1:A:55:ILE:N	0.48	2.24	1	10
1:A:219:TYR:HB2	1:A:275:LEU:HD13	0.48	1.84	5	1
1:A:54:VAL:CG1	1:A:76:ALA:HB1	0.48	2.39	1	10
1:A:122:TRP:CD1	1:A:157:VAL:CG1	0.48	2.95	1	10
1:A:130:ASP:O	1:A:133:PHE:HB3	0.48	2.08	6	1
1:A:193:PHE:CZ	1:A:195:THR:HG21	0.48	2.44	1	10
1:A:311:LEU:HD13	1:A:314:ILE:HG21	0.48	1.86	9	1
1:A:215:MET:SD	1:A:282:PHE:CE2	0.48	3.07	10	1
1:A:64:LEU:N	1:A:64:LEU:HD12	0.47	2.24	1	5
1:A:275:LEU:C	1:A:275:LEU:HD23	0.47	2.29	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:LEU:HD12	1:A:64:LEU:N	0.47	2.24	3	5
1:A:103:ASN:HB2	1:A:188:GLU:CD	0.47	2.29	1	10
1:A:287:LEU:CD1	1:A:291:ILE:HD13	0.47	2.32	1	10
1:A:291:ILE:HD12	1:A:291:ILE:N	0.47	2.24	1	5
1:A:296:HIS:CG	1:A:303:ILE:HD11	0.47	2.44	1	10
1:A:99:TRP:CD1	1:A:101:PHE:HB2	0.47	2.45	1	10
1:A:291:ILE:N	1:A:291:ILE:HD12	0.47	2.24	2	5
1:A:55:ILE:O	1:A:55:ILE:HG13	0.47	2.09	3	1
1:A:122:TRP:HD1	1:A:157:VAL:HG22	0.47	1.66	1	10
1:A:328:ARG:O	1:A:329:SER:C	0.47	2.49	2	2
1:A:122:TRP:HD1	1:A:157:VAL:CG2	0.47	2.22	1	10
1:A:307:VAL:HG12	1:A:311:LEU:HD22	0.47	1.86	1	1
1:A:99:TRP:CD2	1:A:191:CYS:HB3	0.47	2.45	2	10
1:A:210:VAL:CB	1:A:211:PRO:HD3	0.47	2.38	1	10
1:A:55:ILE:O	1:A:55:ILE:CG2	0.47	2.63	8	2
1:A:115:LEU:HD13	1:A:115:LEU:C	0.46	2.31	1	7
1:A:125:CYS:O	1:A:129:VAL:HG23	0.46	2.10	1	10
1:A:201:ILE:O	1:A:205:ILE:HG23	0.46	2.10	1	10
1:A:115:LEU:C	1:A:115:LEU:HD13	0.46	2.31	3	3
1:A:215:MET:SD	1:A:278:ILE:HG21	0.46	2.49	7	3
1:A:288:PRO:HB2	1:A:311:LEU:HD11	0.46	1.86	9	4
1:A:77:VAL:HG13	1:A:78:ALA:N	0.46	2.25	1	10
1:A:311:LEU:HA	1:A:314:ILE:HG13	0.46	1.87	10	3
1:A:133:PHE:CZ	1:A:141:TYR:CD2	0.46	3.03	6	1
1:A:67:VAL:HA	1:A:70:TYR:HD1	0.46	1.66	9	6
1:A:196:ASN:OD1	1:A:198:ALA:HB3	0.46	2.11	1	10
1:A:202:ALA:HA	1:A:205:ILE:HG12	0.46	1.87	1	10
1:A:38:ILE:CD1	1:A:42:LEU:CD1	0.46	2.94	1	10
1:A:66:THR:O	1:A:69:ASN:HB2	0.46	2.11	1	10
1:A:322:ASN:CB	1:A:323:PRO:HD3	0.46	2.41	4	10
1:A:38:ILE:HG23	1:A:39:VAL:N	0.45	2.26	1	10
1:A:121:ILE:CD1	1:A:286:TRP:NE1	0.45	2.74	10	1
1:A:169:ILE:HG23	1:A:174:TYR:CE2	0.45	2.46	1	10
1:A:87:VAL:HG12	1:A:88:PRO:HD3	0.45	1.86	1	10
1:A:101:PHE:HB3	1:A:105:TRP:CD1	0.45	2.46	1	10
1:A:197:GLN:CG	1:A:297:VAL:CG2	0.45	2.94	1	10
1:A:294:ILE:HG22	1:A:298:ILE:CD1	0.45	2.42	1	10
1:A:40:MET:CE	1:A:94:ILE:CD1	0.45	2.95	1	10
1:A:54:VAL:CG1	1:A:76:ALA:CB	0.45	2.95	1	10
1:A:277:ILE:HD11	1:A:325:ILE:HG21	0.45	1.89	10	1
1:A:40:MET:SD	1:A:94:ILE:HD11	0.44	2.52	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ALA:HA	1:A:153:ILE:HD12	0.44	1.87	9	1
1:A:159:ILE:HG23	1:A:160:VAL:N	0.44	2.27	1	10
1:A:87:VAL:HG22	1:A:313:TRP:CH2	0.44	2.47	1	10
1:A:130:ASP:O	1:A:133:PHE:HD2	0.44	1.95	6	1
1:A:52:VAL:O	1:A:55:ILE:O	0.44	2.36	7	1
1:A:171:MET:CG	1:A:173:TRP:NE1	0.44	2.78	1	10
1:A:215:MET:SD	1:A:278:ILE:HG23	0.44	2.53	7	3
1:A:201:ILE:HG12	1:A:202:ALA:N	0.44	2.27	1	10
1:A:32:TRP:NE1	1:A:36:MET:SD	0.44	2.91	1	10
1:A:287:LEU:CD1	1:A:291:ILE:CD1	0.44	2.95	1	10
1:A:38:ILE:HD13	1:A:38:ILE:O	0.44	2.13	1	7
1:A:91:ALA:O	1:A:94:ILE:HG12	0.44	2.12	1	10
1:A:38:ILE:O	1:A:38:ILE:HD13	0.44	2.13	4	3
1:A:89:PHE:CD2	1:A:101:PHE:CE2	0.43	3.06	1	10
1:A:100:THR:HG22	1:A:100:THR:O	0.43	2.13	1	4
1:A:83:GLY:HA2	1:A:87:VAL:CG1	0.43	2.39	1	10
1:A:100:THR:O	1:A:100:THR:HG22	0.43	2.13	4	6
1:A:219:TYR:CD1	1:A:220:SER:N	0.43	2.86	9	1
1:A:208:PHE:CE2	1:A:287:LEU:HD22	0.43	2.49	1	10
1:A:288:PRO:CG	1:A:311:LEU:HD11	0.43	2.43	9	4
1:A:322:ASN:HB2	1:A:323:PRO:HD3	0.43	1.89	10	2
1:A:114:VAL:CG2	1:A:165:SER:CB	0.43	2.95	1	10
1:A:115:LEU:HD11	1:A:158:TRP:HZ3	0.43	1.69	1	10
1:A:219:TYR:CG	1:A:220:SER:N	0.43	2.84	6	3
1:A:219:TYR:CD1	1:A:275:LEU:CD1	0.43	2.96	9	1
1:A:87:VAL:CG2	1:A:313:TRP:CZ3	0.43	3.02	1	10
1:A:87:VAL:HG22	1:A:313:TRP:CZ3	0.43	2.49	1	10
1:A:159:ILE:CG2	1:A:160:VAL:N	0.43	2.81	1	10
1:A:64:LEU:HD23	1:A:332:PHE:CE2	0.43	2.49	10	1
1:A:222:VAL:CG1	1:A:223:PHE:N	0.42	2.82	1	10
1:A:82:MET:CE	1:A:116:CYS:SG	0.42	3.07	1	10
1:A:54:VAL:O	1:A:55:ILE:HD13	0.42	2.15	6	1
1:A:117:VAL:CG1	1:A:118:THR:N	0.42	2.82	1	10
1:A:122:TRP:CD1	1:A:157:VAL:CG2	0.42	2.95	1	10
1:A:52:VAL:CG1	1:A:53:LEU:N	0.42	2.82	1	10
1:A:285:CYS:CA	1:A:314:ILE:HG23	0.42	2.44	9	1
1:A:75:LEU:CD2	1:A:124:LEU:CD2	0.42	2.95	1	10
1:A:55:ILE:O	1:A:55:ILE:CG1	0.42	2.67	3	1
1:A:277:ILE:HD13	1:A:326:TYR:HA	0.42	1.92	9	1
1:A:110:THR:CG2	1:A:111:SER:N	0.42	2.82	1	10
1:A:297:VAL:CG1	1:A:298:ILE:N	0.42	2.83	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:VAL:CG1	1:A:34:VAL:N	0.42	2.82	1	10
1:A:54:VAL:CG1	1:A:55:ILE:N	0.42	2.82	1	10
1:A:288:PRO:CB	1:A:311:LEU:HD11	0.42	2.44	9	4
1:A:286:TRP:HE1	1:A:318:ASN:CB	0.41	2.28	7	1
1:A:291:ILE:N	1:A:291:ILE:CD1	0.41	2.83	1	5
1:A:291:ILE:CD1	1:A:291:ILE:N	0.41	2.83	2	5
1:A:115:LEU:CD1	1:A:158:TRP:CZ3	0.41	2.99	1	10
1:A:93:HIS:CG	1:A:99:TRP:CZ3	0.41	3.08	3	10
1:A:77:VAL:CG1	1:A:78:ALA:N	0.41	2.83	1	10
1:A:115:LEU:HD22	1:A:161:SER:OG	0.41	2.15	1	10
1:A:301:ASN:H	1:A:301:ASN:HD22	0.41	1.57	1	6
1:A:340:LEU:N	1:A:340:LEU:HD12	0.41	2.31	1	4
1:A:340:LEU:HD12	1:A:340:LEU:N	0.41	2.31	3	6
1:A:301:ASN:HD22	1:A:301:ASN:H	0.41	1.57	4	4
1:A:275:LEU:HD23	1:A:276:GLY:CA	0.41	2.44	7	1
1:A:160:VAL:CG1	1:A:161:SER:N	0.41	2.83	1	10
1:A:115:LEU:CG	1:A:166:PHE:HE1	0.41	2.29	1	10
1:A:206:VAL:CG2	1:A:207:SER:N	0.41	2.82	1	10
1:A:210:VAL:HG12	1:A:214:ILE:HD13	0.41	1.93	1	10
1:A:122:TRP:O	1:A:126:VAL:HG23	0.41	2.16	1	10
1:A:189:THR:O	1:A:189:THR:HG22	0.41	2.15	1	6
1:A:122:TRP:CE3	1:A:211:PRO:HG3	0.41	2.51	1	10
1:A:189:THR:HG22	1:A:189:THR:O	0.41	2.15	2	4
1:A:85:ALA:O	1:A:89:PHE:CD1	0.41	2.73	1	10
1:A:311:LEU:HD13	1:A:314:ILE:CG2	0.41	2.45	9	1
1:A:110:THR:HG23	1:A:111:SER:N	0.41	2.30	1	10
1:A:112:ILE:CG2	1:A:113:ASP:N	0.41	2.84	1	10
1:A:287:LEU:HD13	1:A:287:LEU:C	0.41	2.35	1	4
1:A:54:VAL:HG11	1:A:76:ALA:CB	0.41	2.46	1	10
1:A:117:VAL:HG13	1:A:118:THR:N	0.41	2.29	1	10
1:A:287:LEU:C	1:A:287:LEU:HD13	0.41	2.35	2	6
1:A:55:ILE:HD13	1:A:73:THR:HG23	0.41	1.92	3	1
1:A:310:LEU:O	1:A:314:ILE:CG1	0.41	2.69	10	3
1:A:54:VAL:HG13	1:A:55:ILE:HG12	0.41	1.92	10	1
1:A:285:CYS:CB	1:A:314:ILE:C	0.41	2.89	10	1
1:A:202:ALA:CA	1:A:205:ILE:HG12	0.41	2.46	1	10
1:A:181:ALA:O	1:A:185:TYR:CD1	0.40	2.74	1	10
1:A:302:LEU:HA	1:A:302:LEU:HD23	0.40	1.72	1	7
1:A:302:LEU:HD23	1:A:302:LEU:HA	0.40	1.72	3	3
1:A:277:ILE:N	1:A:277:ILE:CD1	0.40	2.82	10	1
1:A:65:GLN:O	1:A:70:TYR:CE1	0.40	2.74	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:219:TYR:CG	1:A:275:LEU:HD13	0.40	2.51	8	2
1:A:115:LEU:CB	1:A:166:PHE:CE1	0.40	3.00	1	10
1:A:275:LEU:O	1:A:275:LEU:HD12	0.40	2.17	5	1
1:A:218:VAL:HG12	1:A:219:TYR:N	0.40	2.31	10	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	256/336 (76%)	245±1 (96±0%)	9±1 (4±0%)	2±1 (1±0%)	24	71
All	All	2560/3360 (76%)	2447 (96%)	93 (4%)	20 (1%)	24	71

All 7 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	286	TRP	10
1	A	133	PHE	3
1	A	326	TYR	2
1	A	150	ALA	2
1	A	55	ILE	1
1	A	141	TYR	1
1	A	327	SER	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	229/296 (77%)	207±2 (90±1%)	22±2 (10±1%)	12	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2290/2960 (77%)	2067 (90%)	223 (10%)	12 57

All 39 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	201	ILE	10
1	A	72	ILE	10
1	A	75	LEU	10
1	A	312	ASN	10
1	A	142	GLN	10
1	A	143	SER	10
1	A	301	ASN	10
1	A	218	VAL	10
1	A	38	ILE	10
1	A	93	HIS	10
1	A	303	ILE	10
1	A	318	ASN	10
1	A	187	GLU	10
1	A	285	CYS	9
1	A	132	TYR	8
1	A	304	ARG	7
1	A	286	TRP	7
1	A	326	TYR	7
1	A	163	LEU	7
1	A	306	GLU	6
1	A	299	GLN	5
1	A	311	LEU	4
1	A	133	PHE	4
1	A	277	ILE	3
1	A	219	TYR	3
1	A	175	ARG	3
1	A	334	CYS	3
1	A	314	ILE	3
1	A	273	LYS	2
1	A	275	LEU	2
1	A	172	HIS	2
1	A	131	ARG	1
1	A	328	ARG	1
1	A	141	TYR	1
1	A	327	SER	1
1	A	167	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	63	ARG	1
1	A	55	ILE	1
1	A	234	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *PeakList.star*

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	38
Number of shifts mapped to atoms	19
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	19
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atoms found in structure. All 19 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	287	LEU	HN	7.81	0.02	1
A	340	LEU	HN	7.77	0.02	1
A	284	LEU	HN	8.39	0.02	1
A	266	CYS	HN	8.11	0.02	1
A	84	LEU	HN	8.13	0.02	1
A	64	LEU	HN	7.88	0.02	1
A	80	LEU	HN	8.9	0.02	1
A	212	LEU	HN	7.95	0.02	1
A	163	LEU	HN	8.65	0.02	1
A	45	LEU	HN	8.23	0.02	1
A	53	LEU	HN	8.01	0.02	1
A	167	LEU	HN	7.15	0.02	1
A	145	LEU	HN	7.61	0.02	1
A	42	LEU	HN	7.96	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	115	LEU	HN	8.64	0.02	1
A	230	LEU	HN	7.85	0.02	1
A	144	LEU	HN	8.04	0.02	1
A	155	LEU	HN	8.21	0.02	1
A	311	LEU	HN	8.31	0.02	1

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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 1%, i.e. 17 atoms were assigned a chemical shift out of a possible 3240. 0 out of 56 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	17/1278 (1%)	0/510 (0%)	0/516 (0%)	17/252 (7%)
Sidechain	0/1563 (0%)	0/903 (0%)	0/607 (0%)	0/53 (0%)
Aromatic	0/399 (0%)	0/209 (0%)	0/173 (0%)	0/17 (0%)
Overall	17/3240 (1%)	0/1622 (0%)	0/1296 (0%)	17/322 (5%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 19 atoms were assigned a chemical shift out of a possible 3932. 0 out of 61 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	19/1546 (1%)	0/617 (0%)	0/624 (0%)	19/305 (6%)
Sidechain	0/1919 (0%)	0/1116 (0%)	0/727 (0%)	0/76 (0%)
Aromatic	0/467 (0%)	0/245 (0%)	0/197 (0%)	0/25 (0%)
Overall	19/3932 (0%)	0/1978 (0%)	0/1548 (0%)	19/406 (5%)

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:

