



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 08:13 am BST

PDB ID : 5OWJ
Title : The dynamic dimer structure of the chaperone Trigger Factor (conformer 2)
Authors : Morgado, L.; Burmann, B.M.; Sharpe, T.; Mazur, A.; Hiller, S.
Deposited on : 2017-09-01

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

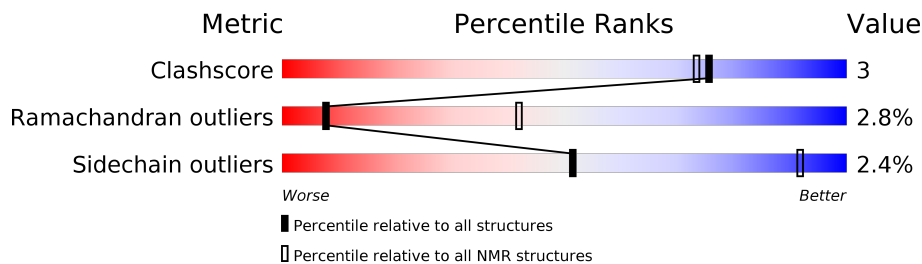
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR



The overall completeness of chemical shifts assignment is 5%.

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	432	 89% 11%
1	B	432	 89% 11%

2 Ensemble composition and analysis i

This entry contains 10 models. Model 9 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:3-A:432, B:1-B:432 (862)	0.93	9

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13582 atoms, of which 6810 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trigger factor.

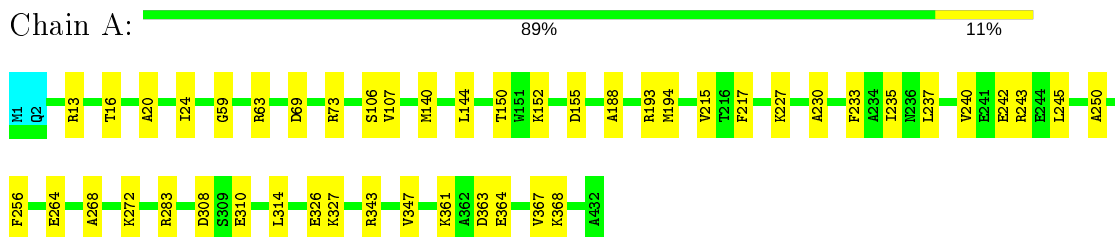
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	432	6791	2119	3405	582	674	11	0
1	B	432	6791	2119	3405	582	674	11	0

4 Residue-property plots

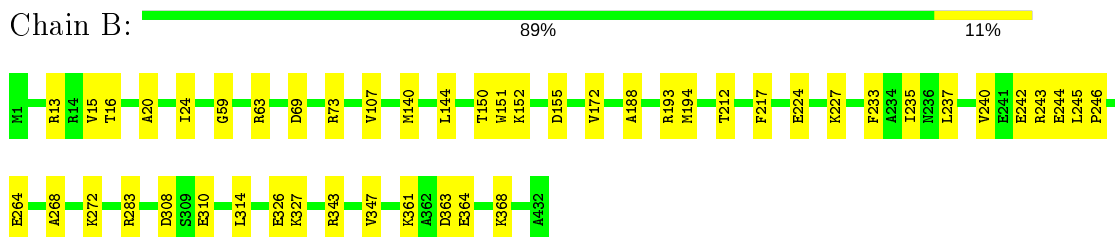
4.1 Average score per residue in the NMR ensemble

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: Trigger factor



- Molecule 1: Trigger factor

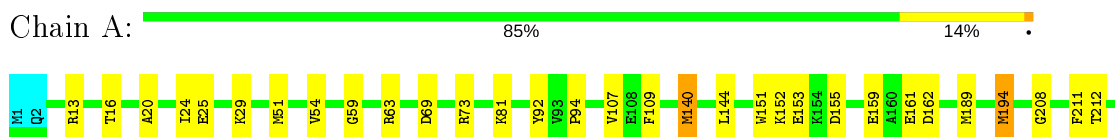


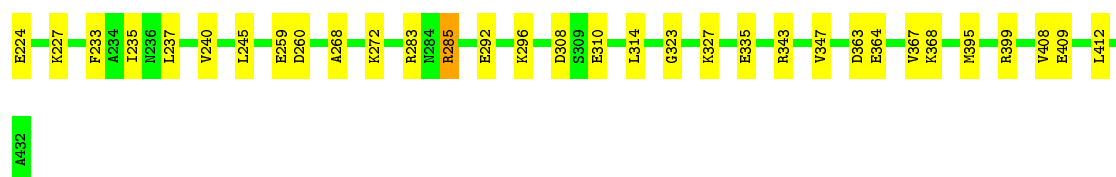
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

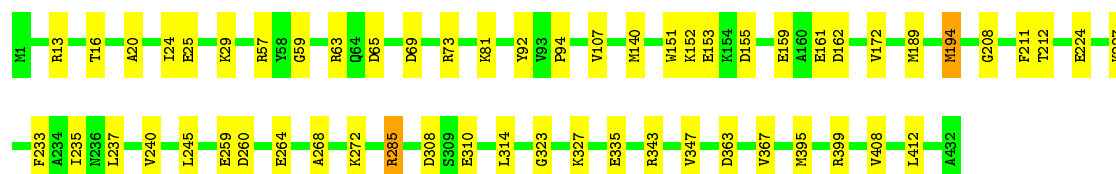
- Molecule 1: Trigger factor





- Molecule 1: Trigger factor

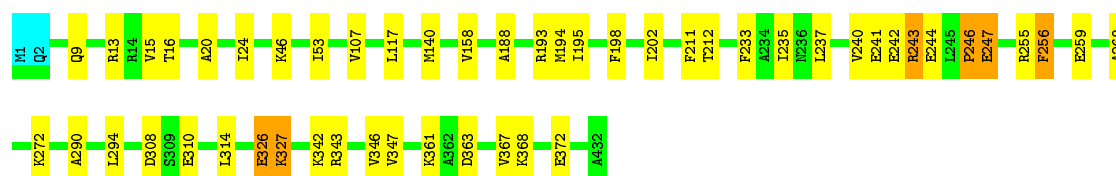
Chain B: 87% 13%



4.2.2 Score per residue for model 2

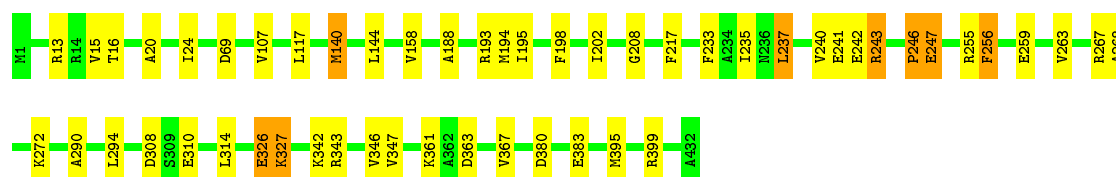
- Molecule 1: Trigger factor

Chain A: 88% 10%



- Molecule 1: Trigger factor

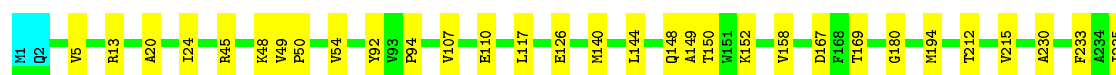
Chain B: 88% 10%



4.2.3 Score per residue for model 3

- Molecule 1: Trigger factor

Chain A: 86% 13%





- Molecule 1: Trigger factor

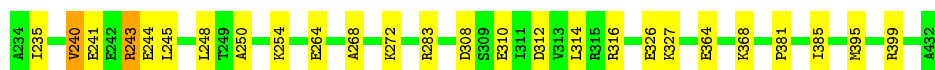
Chain B: 86% 13%



4.2.4 Score per residue for model 4

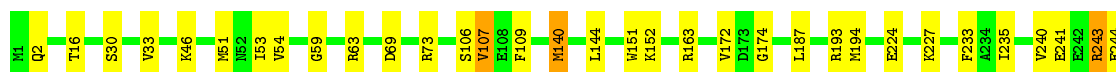
- Molecule 1: Trigger factor

Chain A: 86% 13%



- Molecule 1: Trigger factor

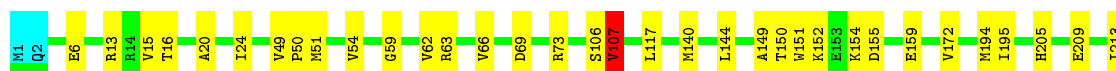
Chain B: 87% 12%



4.2.5 Score per residue for model 5

- Molecule 1: Trigger factor

Chain A: 85% 14%



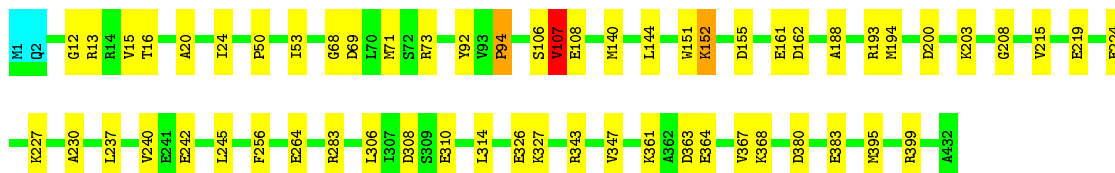
- Molecule 1: Trigger factor



4.2.8 Score per residue for model 8

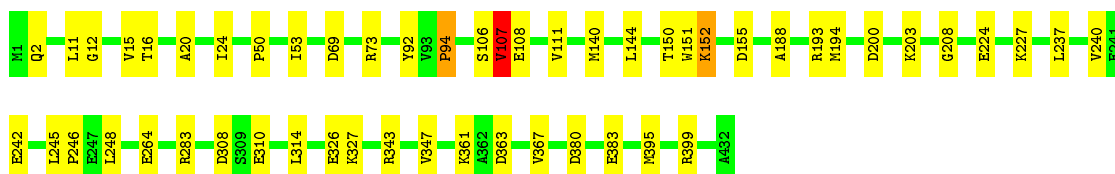
- Molecule 1: Trigger factor

Chain A: 86% 13%



- Molecule 1: Trigger factor

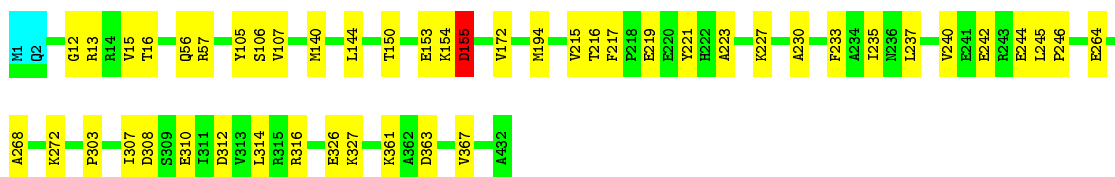
Chain B: 88% 12%



4.2.9 Score per residue for model 9 (medoid)

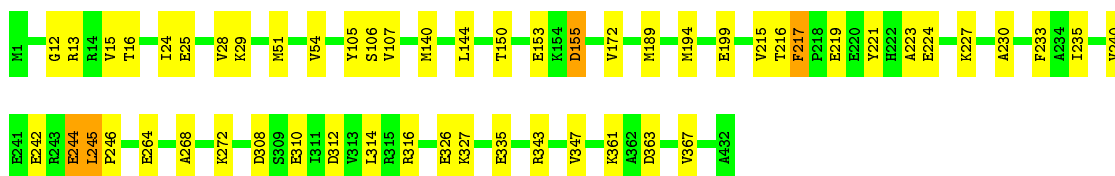
- Molecule 1: Trigger factor

Chain A: 88% 11%



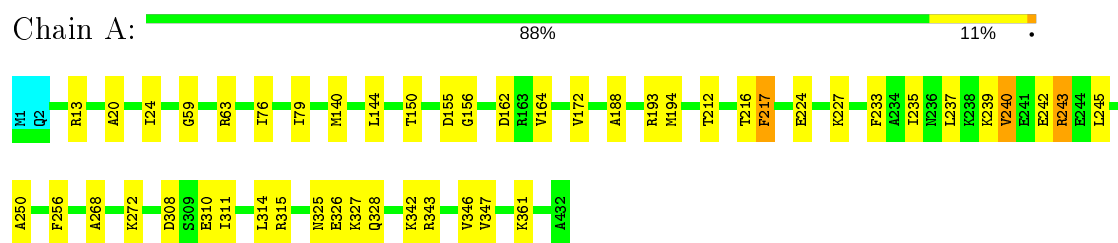
- Molecule 1: Trigger factor

Chain B: 88% 12%

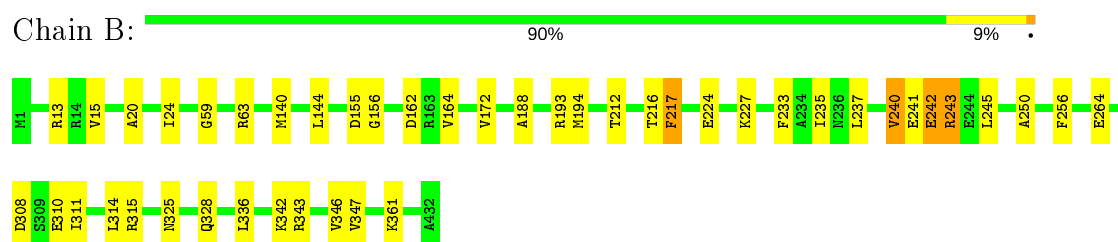


4.2.10 Score per residue for model 10

- Molecule 1: Trigger factor



- Molecule 1: Trigger factor



5 Refinement protocol and experimental data overview

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

Of the 100 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
HADDOCK	structure calculation	
Xplor-NIH	refinement	

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	564
Number of shifts mapped to atoms	564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	5%

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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
1	B	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	316	ARG	Sidechain	1
1	B	316	ARG	Sidechain	1

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	3369	3386	3384	22±5
1	B	3386	3405	3403	22±2
All	All	67550	67910	67870	418

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:161:GLU:HA	1:B:189:MET:O	0.68	1.89	6	2
1:A:161:GLU:HA	1:A:189:MET:O	0.66	1.91	6	2
1:B:69:ASP:O	1:B:73:ARG:HG3	0.65	1.90	6	5
1:A:69:ASP:O	1:A:73:ARG:HG3	0.64	1.92	6	5
1:A:51:MET:HA	1:A:54:VAL:HG22	0.63	1.68	5	1
1:B:326:GLU:O	1:B:327:LYS:HG2	0.63	1.93	3	3
1:B:51:MET:HA	1:B:54:VAL:HG22	0.63	1.70	5	2
1:A:326:GLU:O	1:A:327:LYS:HG2	0.62	1.95	3	4
1:B:188:ALA:HB3	1:B:193:ARG:NH1	0.61	2.09	8	3
1:A:188:ALA:HB3	1:A:193:ARG:NH1	0.61	2.09	8	3
1:A:320:GLN:NE2	1:B:45:ARG:HA	0.58	2.13	3	1
1:A:69:ASP:OD2	1:A:73:ARG:HD2	0.57	1.99	8	5
1:B:140:MET:O	1:B:144:LEU:HG	0.56	2.00	4	9
1:B:20:ALA:O	1:B:24:ILE:HG13	0.56	2.00	7	8
1:A:310:GLU:O	1:A:314:LEU:HG	0.56	2.00	5	8
1:B:59:GLY:O	1:B:63:ARG:HB2	0.56	2.00	4	5
1:B:310:GLU:O	1:B:314:LEU:HG	0.56	2.00	5	8
1:B:200:ASP:O	1:B:203:LYS:HE2	0.56	2.01	8	1
1:A:20:ALA:O	1:A:24:ILE:HG13	0.56	2.00	2	9
1:B:227:LYS:NZ	1:B:336:LEU:HD13	0.55	2.16	6	1
1:B:69:ASP:OD2	1:B:73:ARG:HD2	0.55	2.01	8	5
1:B:290:ALA:O	1:B:294:LEU:HG	0.55	2.02	2	1
1:B:241:GLU:O	1:B:242:GLU:HG2	0.55	2.01	10	1
1:A:364:GLU:O	1:A:368:LYS:HG2	0.55	2.02	3	7
1:B:205:HIS:HA	1:B:209:GLU:OE1	0.54	2.03	5	1
1:B:51:MET:HA	1:B:54:VAL:HG12	0.54	1.78	4	2
1:B:160:ALA:O	1:B:190:GLY:HA3	0.54	2.02	6	1
1:A:59:GLY:O	1:A:63:ARG:HB2	0.54	2.03	5	5
1:A:162:ASP:OD2	1:A:243:ARG:HD3	0.54	2.02	10	1
1:B:92:TYR:O	1:B:94:PRO:HD3	0.54	2.02	1	3
1:A:188:ALA:O	1:A:193:ARG:HG3	0.54	2.02	10	2
1:B:150:THR:OG1	1:B:246:PRO:HA	0.54	2.03	9	2
1:A:193:ARG:NH2	1:B:53:ILE:HD13	0.53	2.18	8	2
1:A:268:ALA:O	1:A:272:LYS:HG2	0.53	2.03	9	8
1:A:243:ARG:O	1:A:243:ARG:HD3	0.53	2.04	3	1
1:B:243:ARG:O	1:B:243:ARG:HD3	0.52	2.04	3	1
1:A:215:VAL:O	1:A:230:ALA:HA	0.52	2.04	3	5
1:A:205:HIS:HA	1:A:209:GLU:OE1	0.52	2.04	5	1
1:A:169:THR:HA	1:A:180:GLY:O	0.52	2.05	3	1
1:B:326:GLU:OE1	1:B:327:LYS:HG3	0.52	2.05	8	1
1:A:140:MET:O	1:A:144:LEU:HG	0.52	2.04	4	9
1:A:253:ILE:HB	1:A:261:GLY:O	0.51	2.04	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:290:ALA:O	1:A:294:LEU:HG	0.51	2.06	2	1
1:A:160:ALA:O	1:A:190:GLY:HA3	0.51	2.06	6	1
1:A:162:ASP:OD1	1:A:164:VAL:HG22	0.51	2.05	10	1
1:A:200:ASP:O	1:A:203:LYS:HE2	0.51	2.05	8	1
1:A:148:GLN:OE1	1:A:255:ARG:HG2	0.51	2.06	3	1
1:A:126:GLU:OE1	1:A:420:LYS:HE3	0.51	2.05	3	1
1:B:169:THR:HA	1:B:180:GLY:O	0.50	2.06	3	1
1:B:215:VAL:O	1:B:230:ALA:HA	0.50	2.05	3	3
1:B:364:GLU:O	1:B:368:LYS:HG2	0.50	2.06	4	5
1:A:193:ARG:NH1	1:B:53:ILE:HG12	0.50	2.21	4	1
1:B:189:MET:HE3	1:B:199:GLU:O	0.50	2.06	9	1
1:B:268:ALA:O	1:B:272:LYS:HG2	0.50	2.07	4	7
1:A:326:GLU:OE1	1:A:327:LYS:HG3	0.50	2.07	8	2
1:B:285:ARG:CG	1:B:285:ARG:HH21	0.49	2.20	1	1
1:B:312:ASP:O	1:B:316:ARG:HG3	0.49	2.07	3	3
1:A:380:ASP:O	1:A:383:GLU:HG2	0.49	2.07	8	1
1:B:224:GLU:O	1:B:227:LYS:HG2	0.49	2.08	4	5
1:A:92:TYR:O	1:A:94:PRO:HD3	0.49	2.07	3	3
1:A:51:MET:HA	1:A:54:VAL:HG12	0.49	1.84	4	2
1:B:162:ASP:OD2	1:B:243:ARG:HD3	0.49	2.06	10	1
1:B:188:ALA:O	1:B:193:ARG:HG3	0.49	2.07	10	1
1:A:312:ASP:O	1:A:316:ARG:HG3	0.49	2.08	3	3
1:B:148:GLN:OE1	1:B:255:ARG:HG2	0.49	2.08	3	1
1:A:6:GLU:O	1:A:13:ARG:HG3	0.49	2.08	5	1
1:A:227:LYS:NZ	1:A:336:LEU:HD13	0.49	2.23	6	1
1:B:195:ILE:H	1:B:195:ILE:HD12	0.49	1.67	2	1
1:A:219:GLU:O	1:A:227:LYS:HE3	0.48	2.07	6	3
1:A:224:GLU:O	1:A:227:LYS:HG2	0.48	2.07	1	2
1:A:150:THR:OG1	1:A:246:PRO:HA	0.48	2.07	9	2
1:A:53:ILE:HD13	1:B:193:ARG:NH2	0.48	2.24	8	2
1:A:45:ARG:HA	1:B:320:GLN:NE2	0.48	2.24	3	1
1:A:216:THR:O	1:A:217:PHE:HB2	0.48	2.08	10	4
1:A:306:LEU:O	1:A:310:GLU:HG2	0.48	2.09	8	1
1:A:106:SER:O	1:A:107:VAL:HG12	0.48	2.07	5	3
1:B:236:ASN:ND2	1:B:238:LYS:HG3	0.48	2.24	7	1
1:A:363:ASP:O	1:A:367:VAL:HG23	0.48	2.09	8	5
1:B:106:SER:O	1:B:107:VAL:HG12	0.48	2.09	5	3
1:A:188:ALA:HB3	1:A:193:ARG:CZ	0.48	2.39	6	1
1:A:53:ILE:HG12	1:B:193:ARG:NH1	0.47	2.24	4	1
1:B:188:ALA:HB3	1:B:193:ARG:CZ	0.47	2.40	6	1
1:A:285:ARG:CG	1:A:285:ARG:HH21	0.47	2.22	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:THR:HG21	1:A:247:GLU:O	0.47	2.10	5	1
1:B:208:GLY:HA2	1:B:237:LEU:O	0.47	2.10	1	2
1:B:12:GLY:HA2	1:B:106:SER:O	0.47	2.10	9	1
1:B:224:GLU:HA	1:B:227:LYS:CD	0.47	2.40	10	1
1:B:156:GLY:HA3	1:B:243:ARG:O	0.47	2.10	10	1
1:A:195:ILE:H	1:A:195:ILE:HD12	0.47	1.69	5	2
1:B:6:GLU:O	1:B:13:ARG:HG3	0.47	2.10	5	1
1:A:159:GLU:HB3	1:A:162:ASP:HB2	0.47	1.87	1	1
1:B:246:PRO:O	1:B:247:GLU:HG2	0.47	2.09	2	1
1:B:216:THR:O	1:B:217:PHE:HB2	0.47	2.10	10	4
1:A:151:TRP:HA	1:A:243:ARG:HA	0.46	1.86	4	2
1:A:408:VAL:O	1:A:412:LEU:HG	0.46	2.10	1	1
1:A:343:ARG:O	1:A:347:VAL:HG23	0.46	2.10	10	8
1:B:408:VAL:O	1:B:412:LEU:HG	0.46	2.09	1	1
1:B:343:ARG:O	1:B:347:VAL:HG23	0.46	2.10	5	8
1:B:253:ILE:HB	1:B:261:GLY:O	0.46	2.11	6	1
1:B:31:GLU:O	1:B:35:VAL:HG23	0.46	2.11	7	1
1:B:259:GLU:HG2	1:B:260:ASP:H	0.46	1.71	1	1
1:A:327:LYS:HE2	1:B:69:ASP:OD1	0.46	2.10	2	1
1:A:211:PHE:O	1:A:212:THR:HB	0.46	2.10	1	2
1:B:395:MET:O	1:B:399:ARG:HG3	0.46	2.11	2	3
1:B:150:THR:HG21	1:B:247:GLU:O	0.46	2.10	5	1
1:A:57:ARG:NH1	1:B:194:MET:SD	0.46	2.89	6	1
1:A:276:ARG:O	1:A:279:LYS:HB3	0.45	2.11	6	2
1:B:195:ILE:HD12	1:B:195:ILE:H	0.45	1.71	5	1
1:A:246:PRO:O	1:A:247:GLU:HG2	0.45	2.11	2	1
1:B:363:ASP:OD2	1:B:365:GLU:HB2	0.45	2.11	6	1
1:A:12:GLY:HA2	1:A:106:SER:O	0.45	2.10	9	1
1:B:126:GLU:OE1	1:B:420:LYS:HE3	0.45	2.11	3	1
1:A:395:MET:O	1:A:399:ARG:HG3	0.45	2.12	1	3
1:B:255:ARG:HG3	1:B:256:PHE:H	0.45	1.72	2	1
1:A:213:ILE:O	1:A:232:LYS:HA	0.45	2.12	5	1
1:A:12:GLY:HA2	1:A:108:GLU:HG2	0.45	1.89	8	1
1:A:283:ARG:HD2	1:A:405:GLU:OE2	0.45	2.12	6	1
1:B:151:TRP:HA	1:B:243:ARG:HA	0.45	1.88	4	2
1:A:236:ASN:ND2	1:A:238:LYS:HG3	0.45	2.27	7	1
1:B:335:GLU:H	1:B:335:GLU:CD	0.45	2.14	1	1
1:B:380:ASP:O	1:B:383:GLU:HG2	0.45	2.10	8	2
1:A:50:PRO:O	1:A:54:VAL:HG13	0.45	2.12	5	1
1:B:311:ILE:O	1:B:315:ARG:HG3	0.44	2.12	6	3
1:A:208:GLY:HA2	1:A:237:LEU:O	0.44	2.12	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:MET:SD	1:B:57:ARG:NH1	0.44	2.90	1	2
1:B:325:ASN:OD1	1:B:328:GLN:HB2	0.44	2.13	10	2
1:B:219:GLU:O	1:B:227:LYS:HE3	0.44	2.12	9	2
1:B:12:GLY:O	1:B:13:ARG:HD3	0.44	2.12	7	1
1:B:162:ASP:OD1	1:B:164:VAL:HG22	0.44	2.12	10	1
1:A:193:ARG:HH11	1:B:53:ILE:HG12	0.44	1.70	4	1
1:B:49:VAL:HG12	1:B:54:VAL:HG12	0.44	1.89	5	1
1:A:239:LYS:O	1:A:240:VAL:HB	0.44	2.13	10	1
1:A:31:GLU:O	1:A:35:VAL:HG23	0.44	2.12	7	1
1:B:363:ASP:O	1:B:367:VAL:HG23	0.44	2.13	9	4
1:A:156:GLY:HA3	1:A:243:ARG:O	0.44	2.13	10	2
1:A:381:PRO:O	1:A:385:ILE:HG13	0.43	2.13	4	1
1:A:224:GLU:HA	1:A:227:LYS:CD	0.43	2.43	6	2
1:A:311:ILE:O	1:A:315:ARG:HG3	0.43	2.13	10	1
1:A:325:ASN:OD1	1:A:328:GLN:HB2	0.43	2.13	3	2
1:B:283:ARG:HD2	1:B:405:GLU:OE2	0.43	2.13	5	2
1:B:50:PRO:O	1:B:54:VAL:HG13	0.43	2.14	5	1
1:A:154:LYS:O	1:A:155:ASP:HB2	0.43	2.12	9	1
1:B:172:VAL:HG23	1:B:177:PHE:CD2	0.43	2.49	6	1
1:B:12:GLY:HA2	1:B:108:GLU:HG2	0.43	1.90	8	1
1:A:255:ARG:HG3	1:A:255:ARG:O	0.43	2.14	3	1
1:A:68:GLY:O	1:A:71:MET:HG2	0.43	2.13	8	1
1:B:212:THR:HA	1:B:233:PHE:O	0.43	2.14	3	1
1:B:335:GLU:CD	1:B:335:GLU:H	0.43	2.16	9	1
1:A:30:SER:O	1:A:33:VAL:HG12	0.43	2.14	4	1
1:A:194:MET:CE	1:A:194:MET:HA	0.43	2.43	7	1
1:A:255:ARG:HG3	1:A:256:PHE:H	0.42	1.74	2	1
1:A:259:GLU:HG2	1:A:260:ASP:H	0.42	1.73	1	1
1:B:285:ARG:CG	1:B:285:ARG:NH2	0.42	2.82	1	1
1:A:368:LYS:O	1:A:372:GLU:HG3	0.42	2.14	2	1
1:B:342:LYS:O	1:B:346:VAL:HG23	0.42	2.14	2	3
1:B:150:THR:HB	1:B:245:LEU:O	0.42	2.14	3	1
1:A:53:ILE:HG12	1:B:193:ARG:HH11	0.42	1.74	4	1
1:B:151:TRP:O	1:B:152:LYS:HB2	0.42	2.15	8	1
1:B:327:LYS:HA	1:B:327:LYS:HE3	0.42	1.91	4	1
1:A:12:GLY:O	1:A:13:ARG:HD3	0.42	2.15	7	1
1:A:292:GLU:OE2	1:A:296:LYS:HE2	0.42	2.14	1	1
1:B:194:MET:HA	1:B:194:MET:CE	0.42	2.43	7	2
1:A:303:PRO:O	1:A:307:ILE:HG13	0.42	2.14	9	1
1:A:194:MET:HA	1:A:194:MET:CE	0.42	2.45	1	1
1:B:25:GLU:O	1:B:29:LYS:HE2	0.42	2.14	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:346:VAL:O	1:A:350:LEU:HG	0.42	2.15	6	1
1:A:49:VAL:HG12	1:A:54:VAL:HB	0.42	1.92	3	1
1:B:255:ARG:O	1:B:255:ARG:HG3	0.42	2.14	3	1
1:A:62:VAL:O	1:A:66:VAL:HG23	0.42	2.15	5	1
1:B:198:PHE:O	1:B:202:ILE:HG12	0.42	2.15	2	1
1:A:154:LYS:HE2	1:A:240:VAL:O	0.42	2.15	4	1
1:A:149:ALA:HB3	1:A:159:GLU:OE1	0.42	2.14	5	1
1:A:307:ILE:O	1:A:311:ILE:HG13	0.41	2.15	5	2
1:B:150:THR:HG22	1:B:151:TRP:H	0.41	1.75	6	1
1:A:151:TRP:O	1:A:152:LYS:HB2	0.41	2.15	8	1
1:B:50:PRO:HG2	1:B:53:ILE:HD12	0.41	1.91	8	1
1:A:151:TRP:O	1:A:152:LYS:HG3	0.41	2.14	1	1
1:A:285:ARG:CG	1:A:285:ARG:NH2	0.41	2.83	1	1
1:A:342:LYS:O	1:A:346:VAL:HG23	0.41	2.15	10	3
1:B:255:ARG:HG3	1:B:256:PHE:N	0.41	2.31	2	1
1:B:224:GLU:CD	1:B:336:LEU:HD12	0.41	2.35	10	1
1:B:211:PHE:O	1:B:212:THR:HB	0.41	2.14	7	2
1:B:252:PHE:CD1	1:B:253:ILE:HG23	0.41	2.51	5	1
1:A:56:GLN:HG3	1:A:57:ARG:HG3	0.41	1.91	9	1
1:A:154:LYS:HG3	1:A:155:ASP:N	0.41	2.31	5	1
1:A:48:LYS:O	1:A:50:PRO:HD3	0.41	2.16	3	1
1:A:198:PHE:O	1:A:202:ILE:HG12	0.41	2.16	2	1
1:A:53:ILE:HG12	1:B:193:ARG:NH2	0.41	2.30	2	1
1:B:263:VAL:O	1:B:267:ARG:HG3	0.41	2.16	2	1
1:B:30:SER:O	1:B:33:VAL:HG12	0.41	2.16	4	1
1:B:276:ARG:O	1:B:279:LYS:HB3	0.41	2.16	7	1
1:A:76:ILE:O	1:A:79:ILE:HG13	0.41	2.16	10	1
1:B:240:VAL:HG12	1:B:242:GLU:H	0.41	1.75	10	1
1:B:151:TRP:O	1:B:152:LYS:HG3	0.41	2.16	1	1
1:A:335:GLU:CD	1:A:335:GLU:H	0.41	2.19	1	1
1:B:241:GLU:HB3	1:B:243:ARG:NH1	0.41	2.30	2	1
1:B:167:ASP:OD1	1:B:183:SER:HA	0.41	2.15	3	1
1:B:266:LEU:O	1:B:270:VAL:HG23	0.41	2.16	5	2
1:A:266:LEU:O	1:A:270:VAL:HG23	0.41	2.16	6	2
1:A:162:ASP:O	1:A:188:ALA:HA	0.41	2.16	8	1
1:A:50:PRO:HG2	1:A:53:ILE:HD12	0.41	1.93	8	1
1:A:161:GLU:OE2	1:A:256:PHE:HA	0.41	2.15	8	1
1:B:150:THR:HG21	1:B:246:PRO:HA	0.41	1.93	8	1
1:A:241:GLU:HB3	1:A:243:ARG:NH1	0.40	2.31	2	1
1:B:173:ASP:OD1	1:B:232:LYS:HE2	0.40	2.16	3	1
1:A:221:TYR:CE2	1:A:223:ALA:HB3	0.40	2.51	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:346:VAL:O	1:B:350:LEU:HG	0.40	2.15	6	1
1:B:11:LEU:HD23	1:B:111:VAL:HG13	0.40	1.93	8	1
1:B:221:TYR:CE2	1:B:223:ALA:HB3	0.40	2.51	9	1
1:A:25:GLU:O	1:A:29:LYS:HE2	0.40	2.17	1	1
1:A:163:ARG:HA	1:A:187:LEU:O	0.40	2.16	4	1
1:B:163:ARG:HA	1:B:187:LEU:O	0.40	2.16	4	1
1:B:149:ALA:HB3	1:B:159:GLU:OE1	0.40	2.15	5	1
1:B:62:VAL:O	1:B:66:VAL:HG23	0.40	2.17	5	1
1:B:24:ILE:O	1:B:28:VAL:HB	0.40	2.17	9	1
1:A:283:ARG:HH12	1:A:409:GLU:HG3	0.40	1.76	1	1
1:B:307:ILE:O	1:B:311:ILE:HG13	0.40	2.16	7	1
1:B:244:GLU:CD	1:B:245:LEU:H	0.40	2.19	9	1
1:B:159:GLU:HB3	1:B:162:ASP:HB2	0.40	1.92	1	1
1:A:4:SER:OG	1:A:17:ILE:HA	0.40	2.17	4	1
1:B:345:VAL:O	1:B:349:LEU:HG	0.40	2.17	4	1
1:B:162:ASP:O	1:B:188:ALA:HA	0.40	2.17	6	1
1:A:49:VAL:HG12	1:A:54:VAL:HG12	0.40	1.93	5	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	429/432 (99%)	390±4 (91±1%)	27±4 (6±1%)	12±2 (3±0%)	8	43
1	B	430/432 (100%)	391±4 (91±1%)	27±3 (6±1%)	12±2 (3±0%)	8	42
All	All	8590/8640 (99%)	7806 (91%)	545 (6%)	239 (3%)	8	42

All 75 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	107	VAL	9
1	A	240	VAL	9
1	B	16	THR	9
1	B	240	VAL	9

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Mol	Chain	Res	Type	Models (Total)
1	B	245	LEU	9
1	A	107	VAL	9
1	A	245	LEU	9
1	A	16	THR	8
1	A	233	PHE	8
1	B	235	ILE	8
1	B	233	PHE	8
1	A	235	ILE	8
1	B	152	LYS	6
1	A	152	LYS	5
1	B	15	VAL	5
1	A	250	ALA	5
1	B	237	LEU	5
1	B	172	VAL	5
1	B	217	PHE	5
1	A	237	LEU	5
1	A	15	VAL	4
1	A	117	LEU	4
1	B	117	LEU	4
1	B	155	ASP	4
1	B	242	GLU	4
1	A	155	ASP	4
1	B	256	PHE	3
1	A	172	VAL	3
1	A	242	GLU	3
1	B	250	ALA	3
1	A	256	PHE	3
1	A	217	PHE	3
1	B	243	ARG	2
1	B	158	VAL	2
1	A	212	THR	2
1	A	5	VAL	2
1	B	248	LEU	2
1	A	158	VAL	2
1	B	5	VAL	2
1	B	212	THR	2
1	A	243	ARG	2
1	A	109	PHE	2
1	A	323	GLY	1
1	B	110	GLU	1
1	A	154	LYS	1
1	A	106	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	B	149	ALA	1
1	A	149	ALA	1
1	B	94	PRO	1
1	A	241	GLU	1
1	A	110	GLU	1
1	B	174	GLY	1
1	B	208	GLY	1
1	A	208	GLY	1
1	B	259	GLU	1
1	A	257	GLY	1
1	B	323	GLY	1
1	B	252	PHE	1
1	A	259	GLU	1
1	B	257	GLY	1
1	A	161	GLU	1
1	B	154	LYS	1
1	A	246	PRO	1
1	B	109	PHE	1
1	A	248	LEU	1
1	B	247	GLU	1
1	B	148	GLN	1
1	A	174	GLY	1
1	B	161	GLU	1
1	B	241	GLU	1
1	A	94	PRO	1
1	B	246	PRO	1
1	A	247	GLU	1
1	A	9	GLN	1
1	A	148	GLN	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	357/359 (99%)	349±2 (98±1%)	8±2 (2±1%)	53 92
1	B	359/359 (100%)	350±2 (98±1%)	9±2 (2±1%)	51 92
All	All	7160/7180 (100%)	6991 (98%)	169 (2%)	51 92

All 61 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	194	MET	10
1	B	194	MET	10
1	B	264	GLU	9
1	B	308	ASP	8
1	A	13	ARG	8
1	A	308	ASP	8
1	B	13	ARG	7
1	A	264	GLU	6
1	B	361	LYS	5
1	B	283	ARG	5
1	B	327	LYS	5
1	B	244	GLU	5
1	A	327	LYS	5
1	A	361	LYS	5
1	A	244	GLU	4
1	A	326	GLU	4
1	B	326	GLU	4
1	A	283	ARG	3
1	B	140	MET	3
1	A	150	THR	3
1	A	242	GLU	2
1	B	107	VAL	2
1	A	153	GLU	2
1	B	153	GLU	2
1	B	243	ARG	2
1	A	46	LYS	2
1	A	107	VAL	2
1	B	2	GLN	2
1	A	140	MET	2
1	A	243	ARG	2
1	B	150	THR	2
1	A	272	LYS	1
1	B	46	LYS	1
1	A	19	ILE	1
1	A	294	LEU	1
1	A	285	ARG	1
1	B	242	GLU	1
1	A	155	ASP	1
1	A	173	ASP	1
1	A	167	ASP	1
1	A	254	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	B	134	ASP	1
1	B	105	TYR	1
1	B	81	LYS	1
1	B	254	LYS	1
1	B	155	ASP	1
1	A	81	LYS	1
1	B	285	ARG	1
1	B	65	ASP	1
1	B	5	VAL	1
1	A	110	GLU	1
1	A	138	ASP	1
1	B	249	THR	1
1	B	19	ILE	1
1	A	388	TYR	1
1	B	251	GLU	1
1	A	5	VAL	1
1	A	105	TYR	1
1	A	335	GLU	1
1	B	388	TYR	1
1	B	110	GLU	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 5% for the well-defined parts and 5% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *TFconv.str*

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	564
Number of shifts mapped to atoms	564
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
$^{13}\text{C}_\alpha$	108	0.72 ± 0.13	Should be applied
$^{13}\text{C}_\beta$	93	1.13 ± 0.21	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	181	-0.52 ± 0.25	Should be applied

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 5%, i.e. 564 atoms were assigned a chemical shift out of a possible 10622. 0 out of 146 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	469/4262 (11%)	180/1700 (11%)	108/1724 (6%)	181/838 (22%)
Sidechain	93/5870 (2%)	0/3405 (0%)	93/2176 (4%)	0/289 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/490 (0%)	1/262 (0%)	0/218 (0%)	1/10 (10%)
Overall	564/10622 (5%)	181/5367 (3%)	201/4118 (5%)	182/1137 (16%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 564 atoms were assigned a chemical shift out of a possible 10650. 0 out of 146 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	469/4272 (11%)	180/1704 (11%)	108/1728 (6%)	181/840 (22%)
Sidechain	93/5888 (2%)	0/3416 (0%)	93/2182 (4%)	0/290 (0%)
Aromatic	2/490 (0%)	1/262 (0%)	0/218 (0%)	1/10 (10%)
Overall	564/10650 (5%)	181/5382 (3%)	201/4128 (5%)	182/1140 (16%)

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:

