



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 08:50 PM BST

PDB ID : 2HAJ
Title : Solution structure of the helicase-binding domain of Escherichia coli primase
Authors : Su, X.C.; Loscha, K.V.; Dixon, N.E.; Otting, G.
Deposited on : 2006-06-13

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

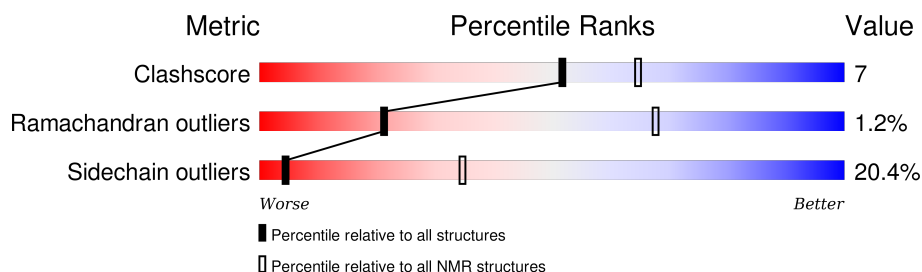
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	148	

2 Ensemble composition and analysis

This entry contains 20 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:451-A:578 (128)	0.58	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 7 single-model clusters were found.

Cluster number	Models
1	2, 5, 9, 11, 14, 17, 19, 20
2	1, 6, 12, 16, 18
Single-model clusters	3; 4; 7; 8; 10; 13; 15

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2167 atoms, of which 1086 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA primase.

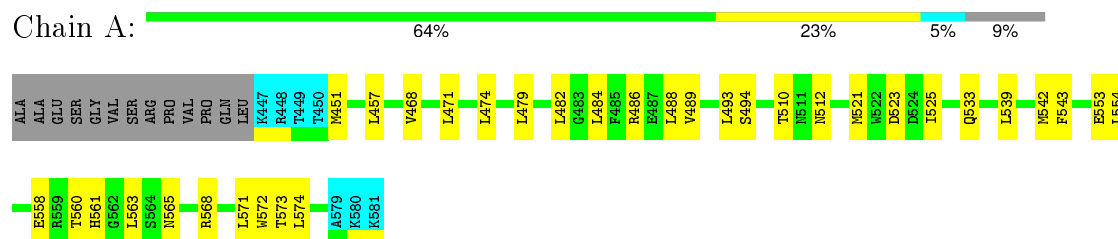
Mol	Chain	Residues	Atoms						Trace
1	A	135	Total	C	H	N	O	S	0
			2167	677	1086	189	211	4	

4 Residue-property plots [i](#)

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: DNA primase

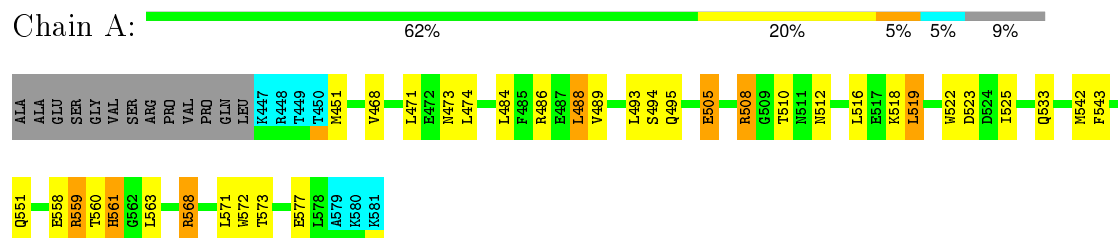


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

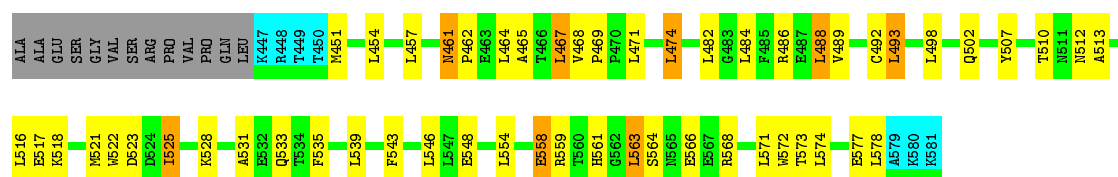
- Molecule 1: DNA primase



4.2.2 Score per residue for model 2

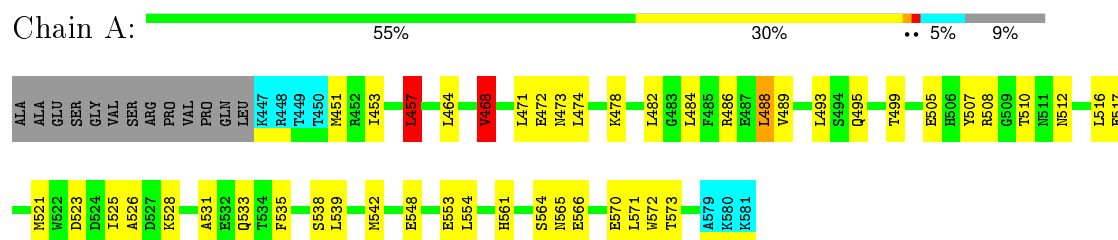
- Molecule 1: DNA primase





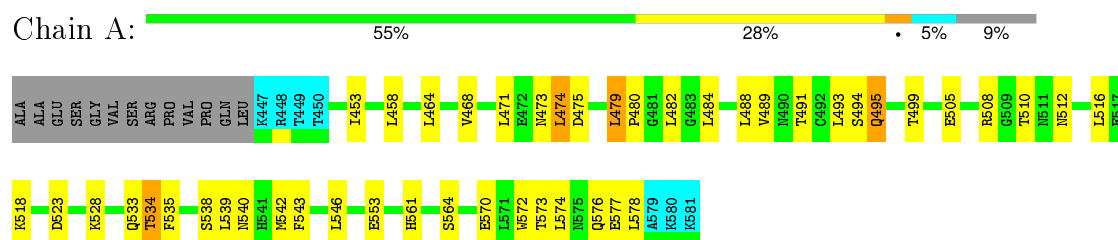
4.2.3 Score per residue for model 3

- Molecule 1: DNA primase



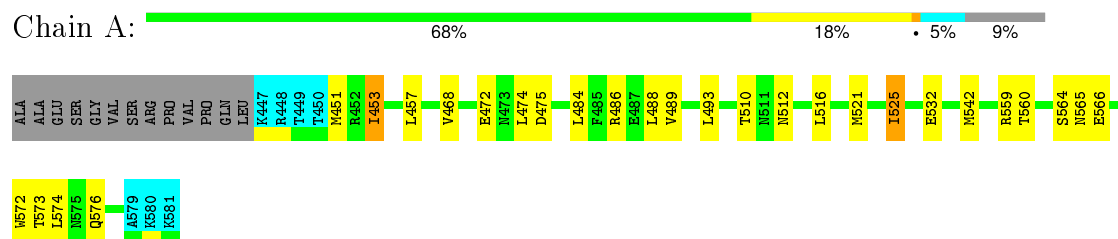
4.2.4 Score per residue for model 4

- Molecule 1: DNA primase



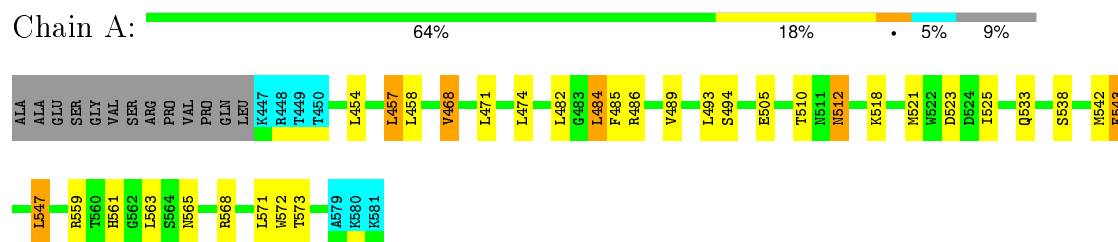
4.2.5 Score per residue for model 5

- Molecule 1: DNA primase



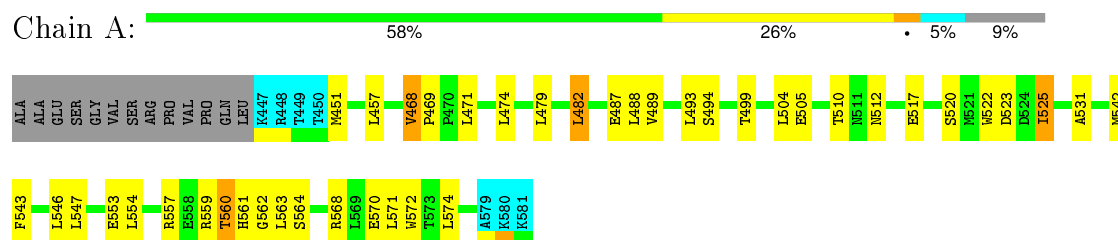
4.2.6 Score per residue for model 6

- Molecule 1: DNA primase



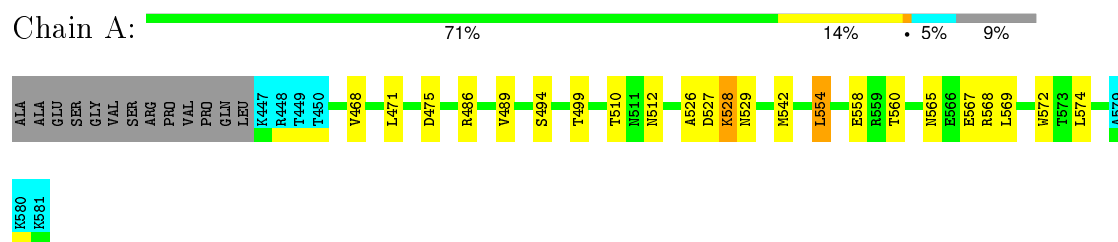
4.2.7 Score per residue for model 7

- Molecule 1: DNA primase



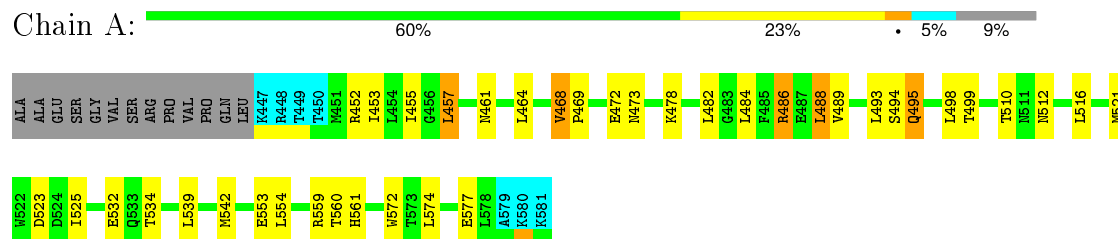
4.2.8 Score per residue for model 8

- Molecule 1: DNA primase



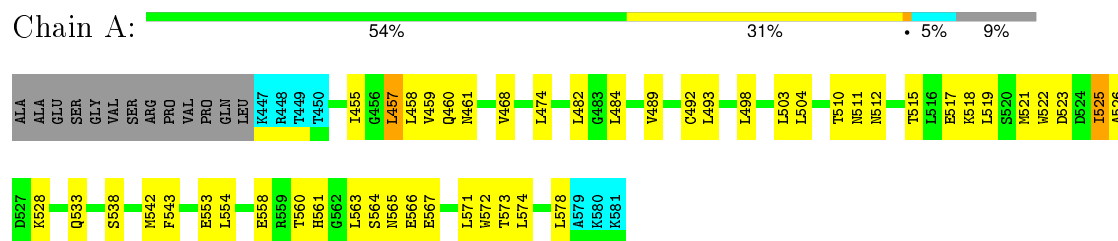
4.2.9 Score per residue for model 9

- Molecule 1: DNA primase



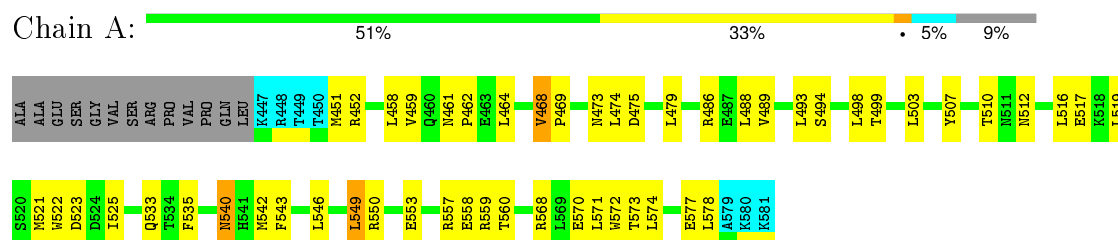
4.2.10 Score per residue for model 10

- Molecule 1: DNA primase



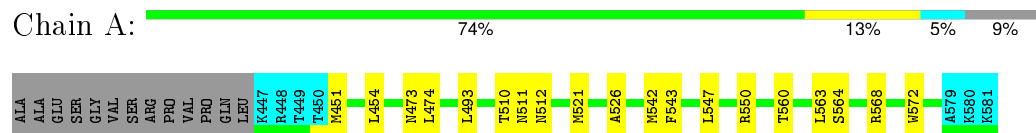
4.2.11 Score per residue for model 11

- Molecule 1: DNA primase



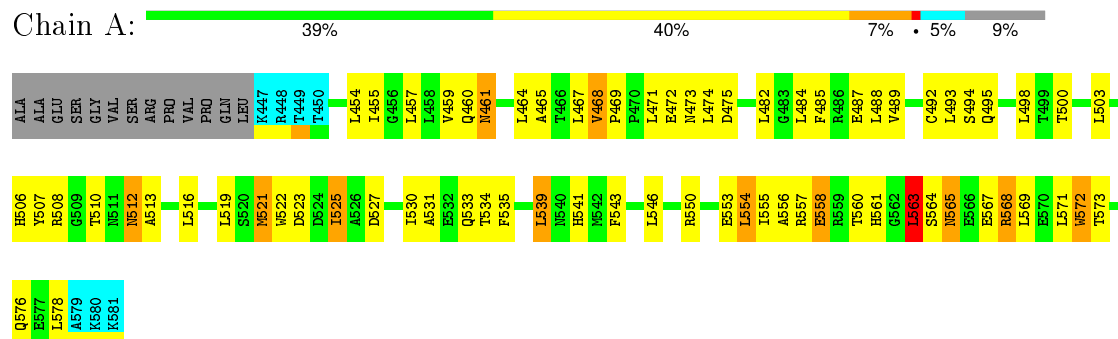
4.2.12 Score per residue for model 12

- Molecule 1: DNA primase



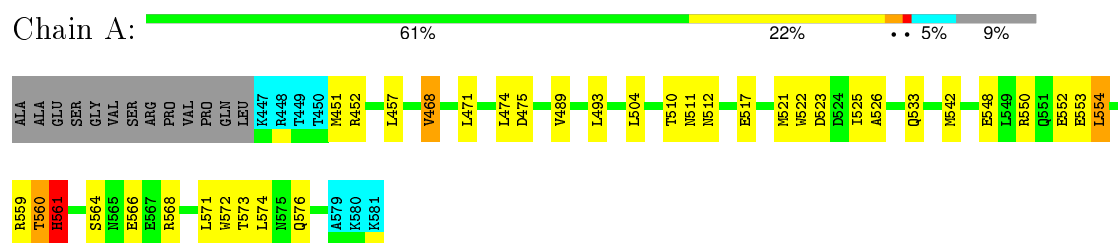
4.2.13 Score per residue for model 13

- Molecule 1: DNA primase



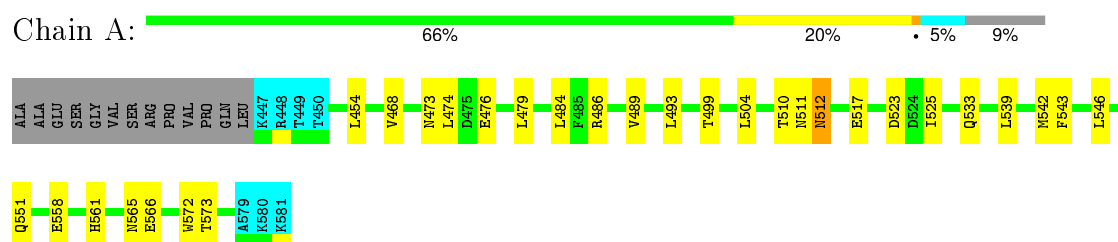
4.2.14 Score per residue for model 14

- Molecule 1: DNA primase



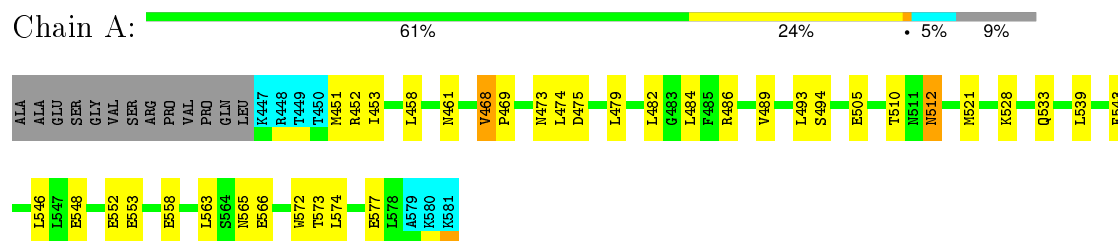
4.2.15 Score per residue for model 15

- Molecule 1: DNA primase



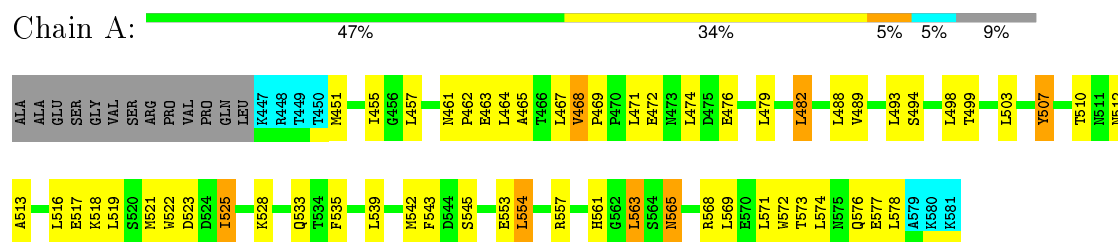
4.2.16 Score per residue for model 16

- Molecule 1: DNA primase



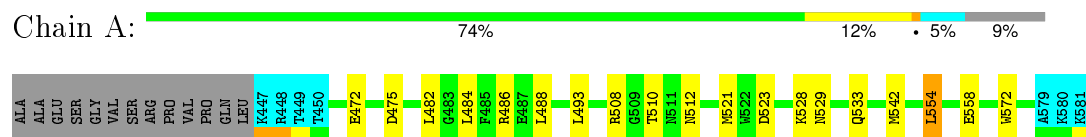
4.2.17 Score per residue for model 17

- Molecule 1: DNA primase



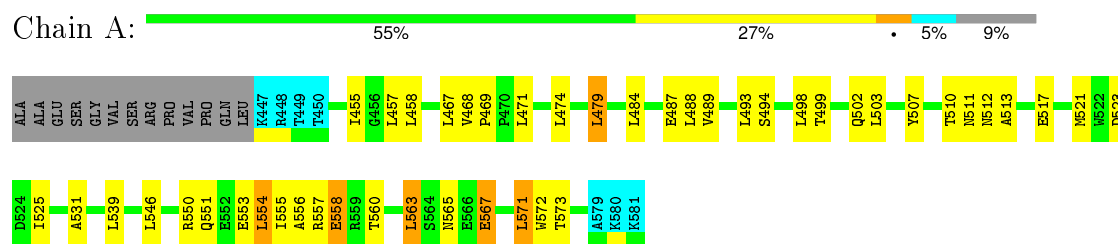
4.2.18 Score per residue for model 18

- Molecule 1: DNA primase



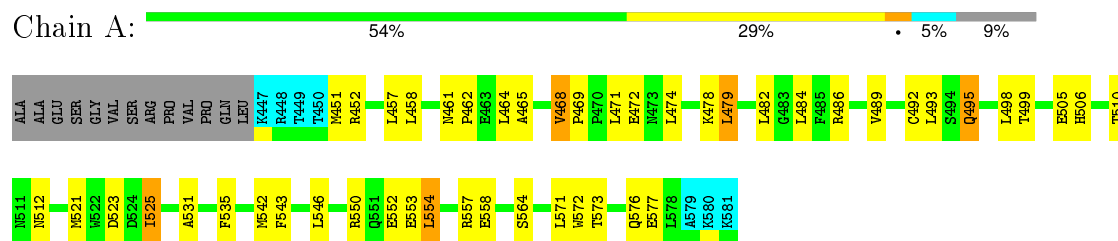
4.2.19 Score per residue for model 19

- Molecule 1: DNA primase



4.2.20 Score per residue for model 20

- Molecule 1: DNA primase



5 Refinement protocol and experimental data overview

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

Of the 200 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	structure solution	2.0
CYANA	refinement	2.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6284
Number of chemical shift lists	2
Total number of shifts	2335
Number of shifts mapped to atoms	2335
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.62±0.04	0±0/1040 (0.0±0.0%)	1.03±0.07	1±1/1413 (0.1±0.1%)
All	All	0.62	0/20800 (0.0%)	1.03	16/28260 (0.1%)

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	0.3±0.5
All	All	0	6

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	486	ARG	NE-CZ-NH2	-7.86	116.37	120.30	6	4
1	A	508	ARG	NE-CZ-NH2	-7.84	116.38	120.30	1	2
1	A	468	VAL	CG1-CB-CG2	-6.71	100.17	110.90	3	1
1	A	519	LEU	CB-CG-CD1	6.18	121.50	111.00	1	1
1	A	457	LEU	CB-CG-CD2	6.00	121.19	111.00	3	1
1	A	550	ARG	NE-CZ-NH1	5.92	123.26	120.30	12	1
1	A	559	ARG	NE-CZ-NH2	-5.68	117.46	120.30	7	1
1	A	547	LEU	CB-CG-CD1	5.51	120.37	111.00	6	1
1	A	534	THR	CA-CB-CG2	5.46	120.04	112.40	4	1
1	A	554	LEU	CB-CA-C	5.43	120.51	110.20	8	1
1	A	452	ARG	NE-CZ-NH2	-5.26	117.67	120.30	9	1
1	A	543	PHE	CB-CG-CD1	5.21	124.45	120.80	6	1

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	486	ARG	Sidechain	1
1	A	507	TYR	Sidechain	1
1	A	538	SER	Mainchain	1
1	A	573	THR	Mainchain	1
1	A	559	ARG	Sidechain	1
1	A	540	ASN	Mainchain	1

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	1024	1018	1021	14±13
All	All	20480	20360	20420	286

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:471:LEU:CD1	1:A:474:LEU:HD12	0.91	1.96	13	1
1:A:488:LEU:HD11	1:A:516:LEU:HD21	0.89	1.44	13	8
1:A:455:ILE:HD13	1:A:484:LEU:HD23	0.88	1.45	19	1
1:A:554:LEU:HD11	1:A:571:LEU:HD21	0.86	1.46	20	1
1:A:457:LEU:HD21	1:A:525:ILE:HG21	0.81	1.50	2	6
1:A:468:VAL:HG11	1:A:489:VAL:HG11	0.78	1.54	14	17
1:A:479:LEU:HD23	1:A:482:LEU:HD13	0.77	1.55	20	1
1:A:488:LEU:CD1	1:A:516:LEU:HD21	0.74	2.12	13	2
1:A:482:LEU:HD13	1:A:482:LEU:O	0.73	1.83	13	1
1:A:555:ILE:HD13	1:A:571:LEU:HD13	0.72	1.60	13	1
1:A:479:LEU:HD21	1:A:546:LEU:HD21	0.71	1.60	11	2
1:A:464:LEU:HD22	1:A:535:PHE:CD2	0.70	2.22	17	4
1:A:471:LEU:HD23	1:A:482:LEU:HD21	0.69	1.62	7	1
1:A:468:VAL:HG22	1:A:469:PRO:HD2	0.69	1.64	13	8
1:A:474:LEU:HD11	1:A:543:PHE:CZ	0.69	2.22	1	4
1:A:457:LEU:CD2	1:A:525:ILE:HD13	0.69	2.17	3	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:543:PHE:HA	1:A:546:LEU:HD12	0.68	1.62	13	3
1:A:555:ILE:CD1	1:A:571:LEU:HD13	0.67	2.20	13	1
1:A:498:LEU:HD21	1:A:503:LEU:HD13	0.67	1.66	13	4
1:A:565:ASN:O	1:A:569:LEU:HD13	0.67	1.88	13	1
1:A:471:LEU:HD12	1:A:482:LEU:HD21	0.67	1.67	20	1
1:A:479:LEU:HD23	1:A:482:LEU:HD23	0.67	1.67	17	1
1:A:507:TYR:O	1:A:513:ALA:HB2	0.66	1.89	13	4
1:A:554:LEU:HD21	1:A:571:LEU:HD11	0.66	1.67	20	2
1:A:471:LEU:HD22	1:A:482:LEU:HD11	0.66	1.66	6	1
1:A:554:LEU:HD11	1:A:571:LEU:CD2	0.65	2.19	20	1
1:A:468:VAL:CG1	1:A:489:VAL:HG11	0.65	2.21	11	8
1:A:554:LEU:HB3	1:A:571:LEU:HD11	0.64	1.68	13	5
1:A:510:THR:HG22	1:A:512:ASN:H	0.64	1.53	17	20
1:A:479:LEU:CD2	1:A:546:LEU:HD21	0.62	2.23	11	2
1:A:474:LEU:HD13	1:A:482:LEU:HD21	0.62	1.70	17	1
1:A:461:ASN:HB3	1:A:464:LEU:HD12	0.62	1.72	2	5
1:A:572:TRP:CD2	1:A:573:THR:N	0.60	2.69	13	1
1:A:554:LEU:HD11	1:A:571:LEU:HD11	0.60	1.73	19	2
1:A:474:LEU:HD21	1:A:543:PHE:CE1	0.59	2.32	20	4
1:A:522:TRP:CE3	1:A:525:ILE:HD11	0.59	2.33	13	6
1:A:572:TRP:CG	1:A:573:THR:N	0.59	2.71	13	1
1:A:572:TRP:CE3	1:A:572:TRP:C	0.59	2.76	13	1
1:A:462:PRO:HB3	1:A:498:LEU:HD23	0.59	1.75	2	4
1:A:469:PRO:O	1:A:471:LEU:HD22	0.58	1.98	13	1
1:A:464:LEU:HD23	1:A:467:LEU:HD13	0.58	1.75	2	1
1:A:482:LEU:C	1:A:482:LEU:HD13	0.58	2.19	13	1
1:A:479:LEU:HD11	1:A:546:LEU:HD21	0.58	1.74	20	1
1:A:465:ALA:O	1:A:468:VAL:HG12	0.57	1.99	2	4
1:A:495:GLN:OE1	1:A:506:HIS:CD2	0.57	2.57	13	1
1:A:457:LEU:HD22	1:A:531:ALA:HB1	0.57	1.75	2	2
1:A:507:TYR:CD2	1:A:516:LEU:CD1	0.57	2.87	2	1
1:A:457:LEU:HD11	1:A:534:THR:HG22	0.57	1.76	13	1
1:A:507:TYR:CD2	1:A:510:THR:HG21	0.56	2.35	2	1
1:A:465:ALA:HB1	1:A:489:VAL:HG13	0.56	1.76	17	1
1:A:557:ARG:C	1:A:563:LEU:HD23	0.55	2.22	13	1
1:A:482:LEU:HD23	1:A:482:LEU:O	0.55	2.00	9	1
1:A:554:LEU:HB2	1:A:571:LEU:HD21	0.54	1.78	2	2
1:A:474:LEU:HD11	1:A:543:PHE:CE1	0.54	2.37	13	2
1:A:479:LEU:HD11	1:A:546:LEU:HD11	0.54	1.78	19	1
1:A:560:THR:HG23	1:A:561:HIS:H	0.54	1.61	14	4
1:A:455:ILE:CG2	1:A:519:LEU:HD13	0.54	2.32	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:554:LEU:HD21	1:A:571:LEU:CD1	0.54	2.31	19	1
1:A:471:LEU:HD13	1:A:474:LEU:HD12	0.54	1.79	13	2
1:A:462:PRO:CB	1:A:498:LEU:HD23	0.53	2.33	2	2
1:A:567:GLU:O	1:A:571:LEU:HD22	0.53	2.04	19	1
1:A:555:ILE:HG12	1:A:571:LEU:HD22	0.52	1.80	13	1
1:A:471:LEU:CD2	1:A:482:LEU:HD11	0.52	2.34	3	2
1:A:454:LEU:HD12	1:A:485:PHE:CZ	0.52	2.40	6	2
1:A:484:LEU:HD13	1:A:488:LEU:HD12	0.51	1.82	2	1
1:A:474:LEU:HD21	1:A:543:PHE:CZ	0.51	2.41	2	4
1:A:464:LEU:HD13	1:A:535:PHE:CD1	0.51	2.41	4	4
1:A:455:ILE:O	1:A:459:VAL:HG23	0.51	2.06	10	1
1:A:471:LEU:HD23	1:A:482:LEU:HD11	0.50	1.82	3	1
1:A:457:LEU:HD22	1:A:531:ALA:CB	0.50	2.35	20	2
1:A:554:LEU:HD12	1:A:554:LEU:C	0.50	2.28	14	2
1:A:451:MET:HE1	1:A:482:LEU:HD12	0.49	1.83	20	1
1:A:464:LEU:HD23	1:A:467:LEU:HD12	0.49	1.82	13	2
1:A:527:ASP:OD2	1:A:530:ILE:HD12	0.49	2.08	13	1
1:A:558:GLU:OE2	1:A:568:ARG:CG	0.48	2.60	13	1
1:A:491:THR:HG22	1:A:495:GLN:HE22	0.48	1.66	4	1
1:A:569:LEU:O	1:A:572:TRP:CD1	0.48	2.67	13	1
1:A:554:LEU:C	1:A:554:LEU:HD12	0.48	2.29	20	1
1:A:465:ALA:CB	1:A:489:VAL:HG13	0.48	2.38	17	1
1:A:468:VAL:HG23	1:A:539:LEU:HD11	0.48	1.85	13	1
1:A:484:LEU:HD11	1:A:512:ASN:HD21	0.48	1.68	6	1
1:A:479:LEU:HD13	1:A:482:LEU:HG	0.48	1.85	4	1
1:A:465:ALA:HB1	1:A:493:LEU:HD23	0.48	1.84	2	1
1:A:464:LEU:HD13	1:A:535:PHE:CD2	0.48	2.44	20	1
1:A:572:TRP:C	1:A:572:TRP:CD2	0.48	2.87	13	1
1:A:549:LEU:HD23	1:A:550:ARG:N	0.48	2.24	11	1
1:A:457:LEU:HD11	1:A:534:THR:CG2	0.47	2.39	13	1
1:A:522:TRP:CE3	1:A:525:ILE:CD1	0.47	2.97	17	3
1:A:455:ILE:HG22	1:A:519:LEU:HD13	0.47	1.86	17	2
1:A:455:ILE:O	1:A:459:VAL:N	0.47	2.47	13	1
1:A:565:ASN:O	1:A:569:LEU:CD1	0.46	2.62	13	1
1:A:471:LEU:HG	1:A:474:LEU:HD12	0.46	1.86	19	2
1:A:504:LEU:HD21	1:A:517:GLU:HA	0.46	1.87	10	3
1:A:556:ALA:O	1:A:560:THR:CG2	0.46	2.63	13	1
1:A:492:CYS:SG	1:A:498:LEU:HD22	0.46	2.50	2	1
1:A:574:LEU:CD1	1:A:578:LEU:HD12	0.46	2.40	17	1
1:A:464:LEU:HB3	1:A:535:PHE:CZ	0.46	2.46	13	1
1:A:453:ILE:HD12	1:A:534:THR:CG2	0.46	2.41	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:474:LEU:HD11	1:A:543:PHE:HE1	0.45	1.69	13	1
1:A:455:ILE:CD1	1:A:484:LEU:HD23	0.45	2.33	19	1
1:A:574:LEU:HD13	1:A:574:LEU:O	0.45	2.11	17	1
1:A:554:LEU:CD1	1:A:571:LEU:HD21	0.45	2.32	20	1
1:A:457:LEU:CD2	1:A:457:LEU:N	0.45	2.79	9	1
1:A:469:PRO:O	1:A:471:LEU:HD12	0.45	2.11	7	1
1:A:474:LEU:HD21	1:A:543:PHE:CD1	0.45	2.46	7	1
1:A:479:LEU:HG	1:A:546:LEU:HD21	0.45	1.89	15	1
1:A:458:LEU:HD11	1:A:492:CYS:SG	0.45	2.51	20	2
1:A:488:LEU:HD11	1:A:516:LEU:CD2	0.45	2.32	13	1
1:A:505:GLU:OE1	1:A:508:ARG:HD3	0.45	2.12	1	1
1:A:484:LEU:CD1	1:A:488:LEU:HD12	0.44	2.41	2	1
1:A:457:LEU:O	1:A:461:ASN:N	0.44	2.50	13	1
1:A:464:LEU:HD22	1:A:535:PHE:CG	0.44	2.47	17	1
1:A:568:ARG:HA	1:A:571:LEU:HD12	0.43	1.89	1	2
1:A:459:VAL:HG12	1:A:460:GLN:OE1	0.43	2.12	10	1
1:A:468:VAL:HG21	1:A:485:PHE:CE2	0.43	2.48	13	1
1:A:507:TYR:CD2	1:A:516:LEU:HD13	0.43	2.49	17	3
1:A:504:LEU:HD21	1:A:520:SER:HB2	0.43	1.91	7	1
1:A:471:LEU:HA	1:A:474:LEU:HD13	0.43	1.89	1	1
1:A:482:LEU:C	1:A:482:LEU:CD1	0.43	2.87	13	1
1:A:512:ASN:OD1	1:A:512:ASN:N	0.43	2.50	13	1
1:A:504:LEU:HD21	1:A:517:GLU:CA	0.43	2.43	10	1
1:A:457:LEU:HD22	1:A:525:ILE:HD13	0.43	1.90	3	1
1:A:471:LEU:HD12	1:A:474:LEU:HD12	0.43	1.82	13	1
1:A:479:LEU:HD21	1:A:546:LEU:HD11	0.43	1.91	7	1
1:A:563:LEU:HD12	1:A:567:GLU:CB	0.42	2.44	13	1
1:A:453:ILE:HG23	1:A:457:LEU:CD1	0.42	2.44	5	1
1:A:558:GLU:HB2	1:A:563:LEU:HD12	0.42	1.91	19	1
1:A:558:GLU:HB2	1:A:563:LEU:HD21	0.42	1.89	13	1
1:A:558:GLU:HB2	1:A:563:LEU:HD11	0.42	1.91	2	1
1:A:464:LEU:HD13	1:A:535:PHE:CG	0.42	2.50	13	1
1:A:457:LEU:HD22	1:A:525:ILE:CD1	0.42	2.45	9	1
1:A:457:LEU:HD13	1:A:531:ALA:O	0.42	2.14	13	1
1:A:495:GLN:HB3	1:A:498:LEU:HD13	0.42	1.92	9	1
1:A:457:LEU:CD1	1:A:531:ALA:HB1	0.42	2.45	3	1
1:A:455:ILE:HG23	1:A:488:LEU:HD13	0.42	1.90	9	1
1:A:554:LEU:HD11	1:A:571:LEU:CD1	0.41	2.45	14	1
1:A:459:VAL:HA	1:A:503:LEU:HD22	0.41	1.90	11	1
1:A:527:ASP:CG	1:A:528:LYS:H	0.41	2.18	8	1
1:A:454:LEU:HD23	1:A:535:PHE:CE1	0.41	2.50	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:565:ASN:O	1:A:569:LEU:HD23	0.41	2.16	17	1
1:A:469:PRO:HD2	1:A:539:LEU:HD11	0.41	1.93	19	1
1:A:519:LEU:HD22	1:A:522:TRP:CE3	0.41	2.51	11	1
1:A:468:VAL:CG2	1:A:469:PRO:HD2	0.40	2.42	13	1
1:A:521:MET:O	1:A:522:TRP:C	0.40	2.59	13	1
1:A:453:ILE:HG21	1:A:538:SER:HB2	0.40	1.93	3	1
1:A:468:VAL:HG11	1:A:489:VAL:CG1	0.40	2.42	13	1
1:A:492:CYS:SG	1:A:498:LEU:CD2	0.40	3.09	13	1
1:A:495:GLN:HE22	1:A:506:HIS:CD2	0.40	2.35	20	1
1:A:460:GLN:O	1:A:500:THR:OG1	0.40	2.40	13	1
1:A:556:ALA:O	1:A:560:THR:HG22	0.40	2.17	19	1
1:A:515:THR:HG22	1:A:519:LEU:HD11	0.40	1.93	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	128/148 (86%)	117±2 (91±1%)	9±2 (7±2%)	2±1 (1±1%)	21	68
All	All	2560/2960 (86%)	2341 (91%)	189 (7%)	30 (1%)	21	68

All 12 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	475	ASP	8
1	A	526	ALA	5
1	A	451	MET	3
1	A	563	LEU	3
1	A	476	GLU	2
1	A	525	ILE	2
1	A	495	GLN	2
1	A	561	HIS	1
1	A	562	GLY	1
1	A	472	GLU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	474	LEU	1
1	A	480	PRO	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	115/131 (88%)	92±5 (80±5%)	23±5 (20±5%)	4	35
All	All	2300/2620 (88%)	1831 (80%)	469 (20%)	4	35

All 74 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	572	TRP	20
1	A	493	LEU	19
1	A	523	ASP	16
1	A	542	MET	16
1	A	521	MET	15
1	A	533	GLN	13
1	A	573	THR	13
1	A	553	GLU	12
1	A	484	LEU	12
1	A	494	SER	11
1	A	558	GLU	11
1	A	564	SER	10
1	A	499	THR	10
1	A	561	HIS	10
1	A	574	LEU	10
1	A	565	ASN	10
1	A	468	VAL	10
1	A	473	ASN	9
1	A	568	ARG	9
1	A	563	LEU	9
1	A	577	GLU	8
1	A	486	ARG	8
1	A	539	LEU	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	554	LEU	8
1	A	488	LEU	8
1	A	528	LYS	8
1	A	525	ILE	8
1	A	505	GLU	7
1	A	566	GLU	7
1	A	560	THR	7
1	A	451	MET	7
1	A	559	ARG	7
1	A	517	GLU	6
1	A	472	GLU	6
1	A	576	GLN	6
1	A	518	LYS	6
1	A	482	LEU	5
1	A	461	ASN	5
1	A	557	ARG	5
1	A	511	ASN	5
1	A	458	LEU	5
1	A	578	LEU	4
1	A	570	GLU	4
1	A	452	ARG	4
1	A	457	LEU	4
1	A	512	ASN	4
1	A	550	ARG	4
1	A	548	GLU	3
1	A	508	ARG	3
1	A	471	LEU	3
1	A	547	LEU	3
1	A	479	LEU	3
1	A	487	GLU	3
1	A	551	GLN	3
1	A	567	GLU	3
1	A	552	GLU	3
1	A	478	LYS	3
1	A	474	LEU	3
1	A	495	GLN	3
1	A	532	GLU	2
1	A	529	ASN	2
1	A	571	LEU	2
1	A	522	TRP	2
1	A	454	LEU	2
1	A	540	ASN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	502	GLN	2
1	A	467	LEU	2
1	A	453	ILE	2
1	A	545	SER	1
1	A	549	LEU	1
1	A	519	LEU	1
1	A	569	LEU	1
1	A	463	GLU	1
1	A	555	ILE	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 84% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6284

Chemical shift list name: *assigned_chem_shift_list_1*

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	915
Number of shifts mapped to atoms	915
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
$^{13}\text{C}_\alpha$	147	-0.62 ± 0.10	Should be applied
$^{13}\text{C}_\beta$	132	0.12 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	146	-0.38 ± 0.09	None needed (< 0.5 ppm)
^{15}N	140	0.11 ± 0.29	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 49%, i.e. 794 atoms were assigned a chemical shift out of a possible 1606. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	626/630 (99%)	250/251 (100%)	253/256 (99%)	123/123 (100%)
Sidechain	164/896 (18%)	32/519 (6%)	116/337 (34%)	16/40 (40%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	4/80 (5%)	2/43 (5%)	0/32 (0%)	2/5 (40%)
Overall	794/1606 (49%)	284/813 (35%)	369/625 (59%)	141/168 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 835 atoms were assigned a chemical shift out of a possible 1708. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	661/665 (99%)	264/265 (100%)	267/270 (99%)	130/130 (100%)
Sidechain	170/963 (18%)	32/559 (6%)	122/358 (34%)	16/46 (35%)
Aromatic	4/80 (5%)	2/43 (5%)	0/32 (0%)	2/5 (40%)
Overall	835/1708 (49%)	298/867 (34%)	389/660 (59%)	148/181 (82%)

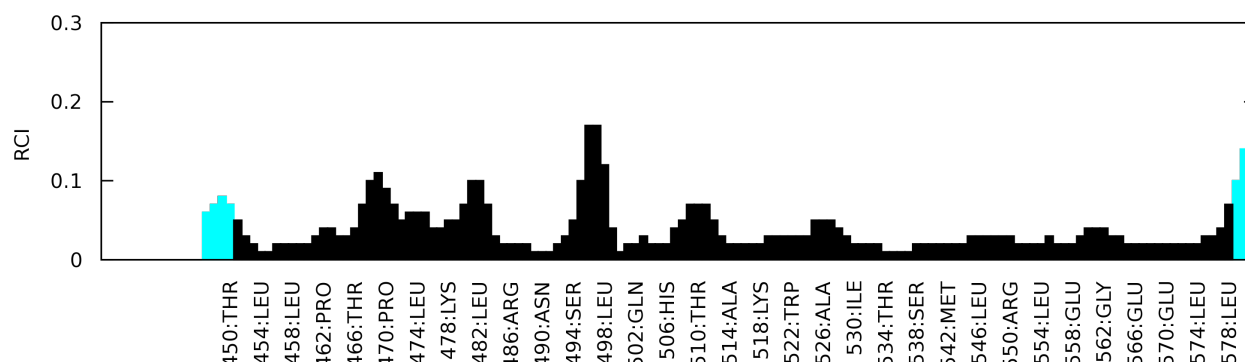
7.1.4 Statistically unusual chemical shifts [i](#)

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:



7.2 Chemical shift list 2

File name: BMRB entry 6284

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	1420
Number of shifts mapped to atoms	1420
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

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	111	-0.66 ± 0.13	Should be applied
$^{13}\text{C}_\beta$	113	0.21 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	140	0.12 ± 0.29	None needed (< 0.5 ppm)

7.2.3 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 73%, i.e. 1169 atoms were assigned a chemical shift out of a possible 1606. 27 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	483/630 (77%)	251/251 (100%)	109/256 (43%)	123/123 (100%)
Sidechain	653/896 (73%)	441/519 (85%)	211/337 (63%)	1/40 (2%)
Aromatic	33/80 (41%)	33/43 (77%)	0/32 (0%)	0/5 (0%)
Overall	1169/1606 (73%)	725/813 (89%)	320/625 (51%)	124/168 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1191 atoms were assigned a chemical shift out of a possible 1708. 27 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	501/665 (75%)	260/265 (98%)	111/270 (41%)	130/130 (100%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Sidechain	657/963 (68%)	443/559 (79%)	213/358 (59%)	1/46 (2%)
Aromatic	33/80 (41%)	33/43 (77%)	0/32 (0%)	0/5 (0%)
Overall	1191/1708 (70%)	736/867 (85%)	324/660 (49%)	131/181 (72%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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:

