Full wwPDB NMR Structure Validation Report (i)

Jan 11, 2021 – 02:13 PM EST

PDB ID	:	6BGH
Title	:	Solution NMR structure of Brd3 ET domain bound to Brg1 peptide
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Deposited on	:	2017-10-28

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 (i) symbol.

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

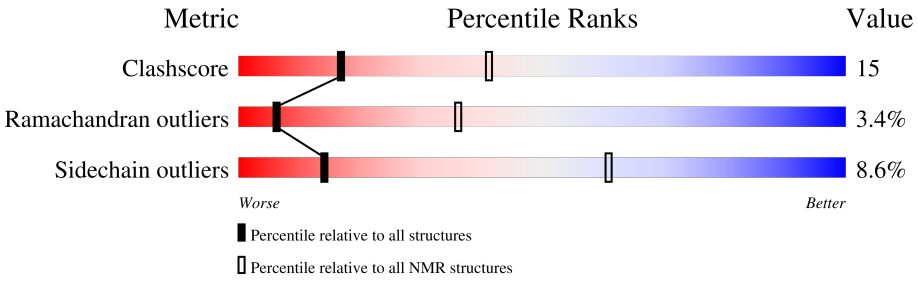
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.16
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	87	55% 21% • 23%
2	B	12	8% 33% 17% 42%

2 Ensemble composition and analysis

This entry contains 20 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:572-A:638, B:1593-B:1599 (74)	0.69	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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1647 atoms, of which 836 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bromodomain-containing protein 3.

Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1423	438	710	126	147	2	

- Molecule 2 is a protein called Brd3_ET.

Mol	Chain	Residues	Atoms					Trace
2	B	12	Total	C	H	N	O	0
			224	63	126	22	13	

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

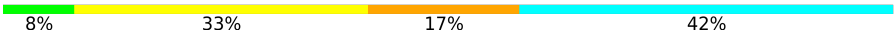
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Bromodomain-containing protein 3

Chain A:

• Molecule 2: Brd3_ET

Chain B:



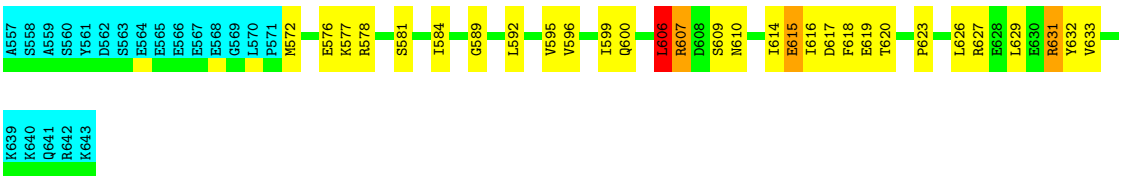
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

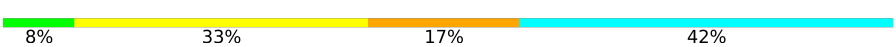
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

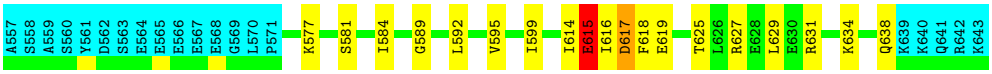
Chain B:



4.2.2 Score per residue for model 2

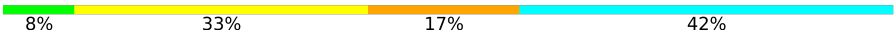
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

Chain B:



4.2.3 Score per residue for model 3

• Molecule 1: Bromodomain-containing protein 3

Chain A:

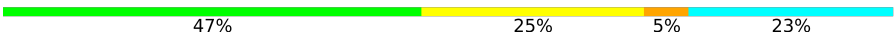
• Molecule 2: Brd3_ET

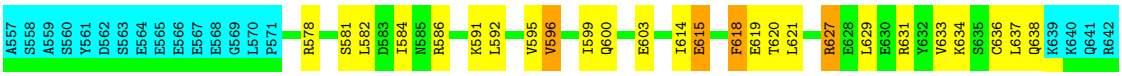
Chain B:

4.2.4 Score per residue for model 4

• Molecule 1: Bromodomain-containing protein 3

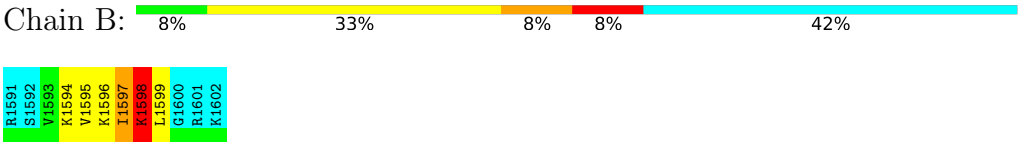
Chain A:





• Molecule 2: Brd3_ET

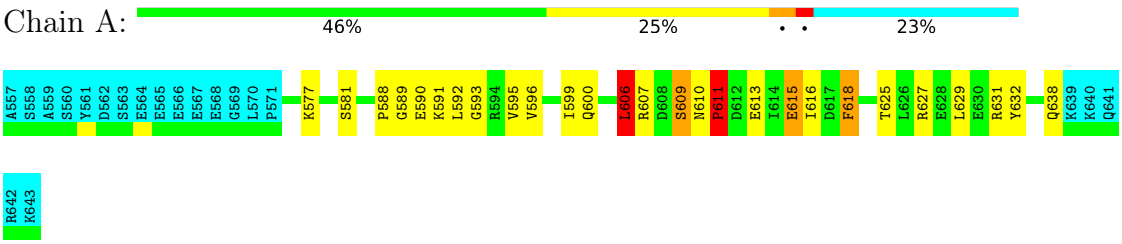
Chain B:



4.2.5 Score per residue for model 5

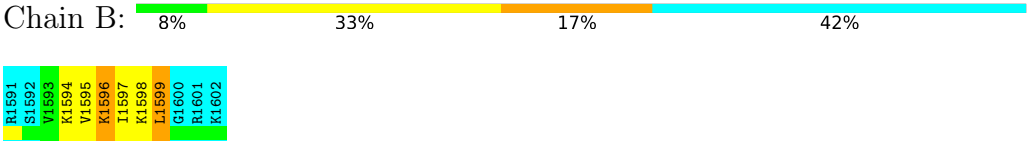
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

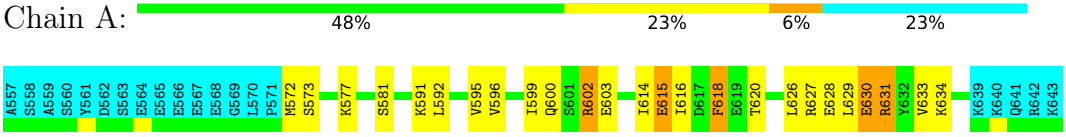
Chain B:



4.2.6 Score per residue for model 6

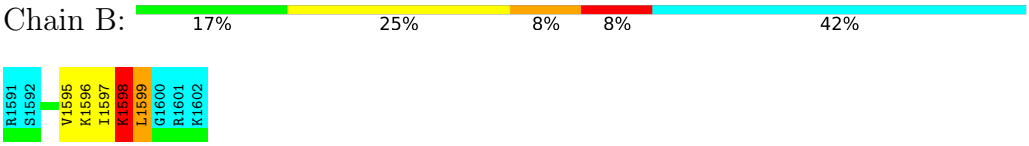
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

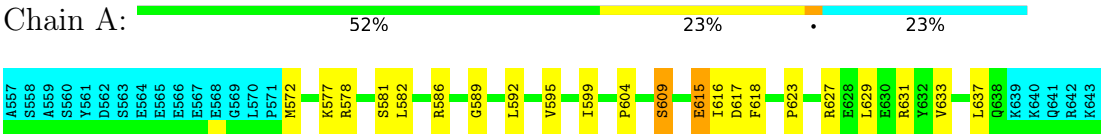
Chain B:



4.2.7 Score per residue for model 7

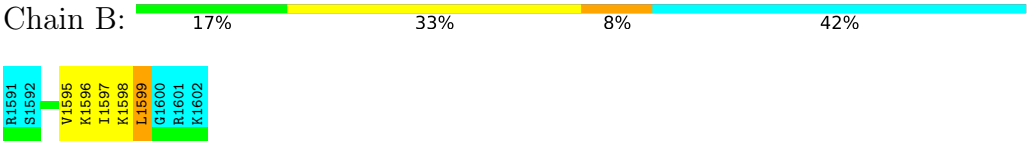
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

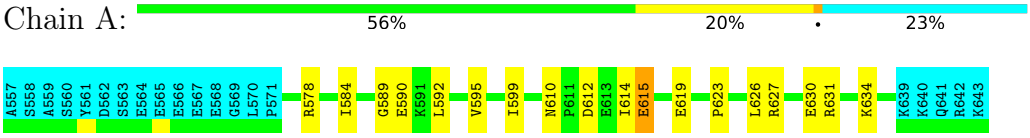
Chain B:



4.2.8 Score per residue for model 8

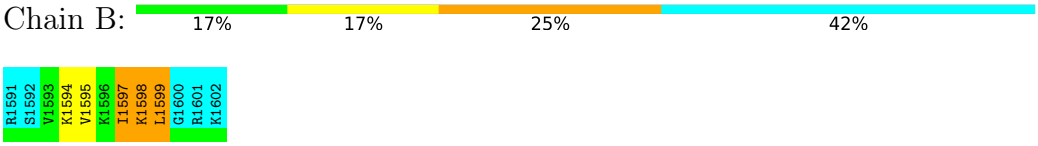
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

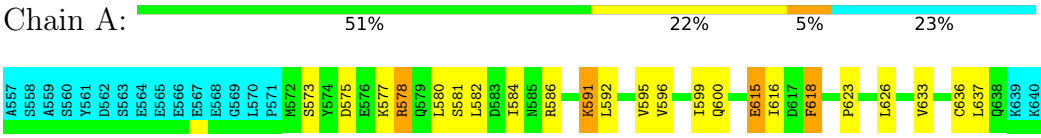
Chain B:



4.2.9 Score per residue for model 9 (medoid)

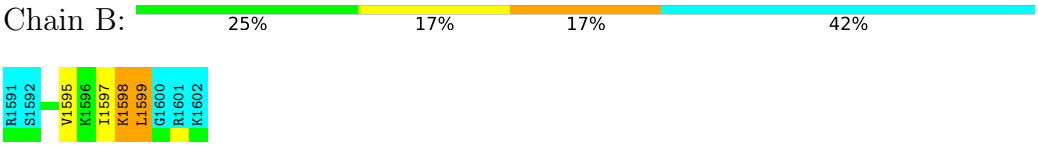
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

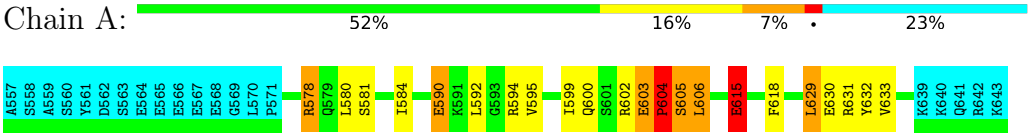
Chain B:



4.2.10 Score per residue for model 10

• Molecule 1: Bromodomain-containing protein 3

Chain A:



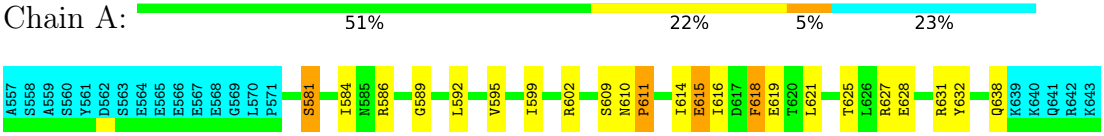
• Molecule 2: Brd3_ET

Chain B:

4.2.11 Score per residue for model 11

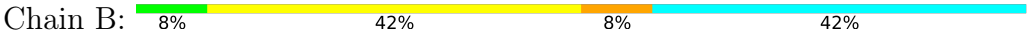
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

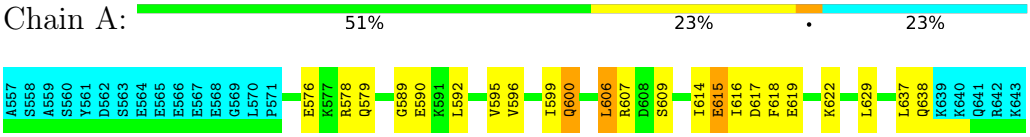
Chain B:



4.2.12 Score per residue for model 12

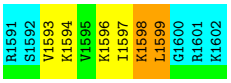
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

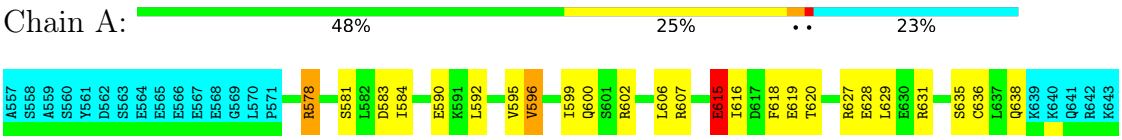
Chain B:



4.2.13 Score per residue for model 13

• Molecule 1: Bromodomain-containing protein 3

Chain A:



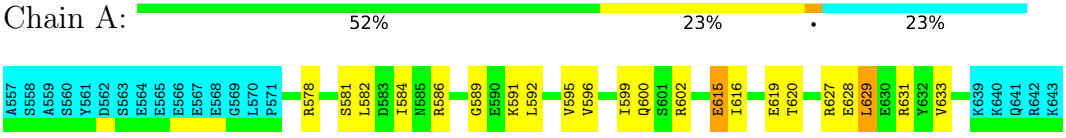
• Molecule 2: Brd3_ET

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: Bromodomain-containing protein 3

Chain A:



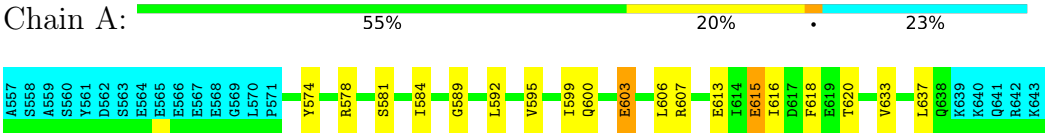
• Molecule 2: Brd3_ET

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: Bromodomain-containing protein 3

Chain A:



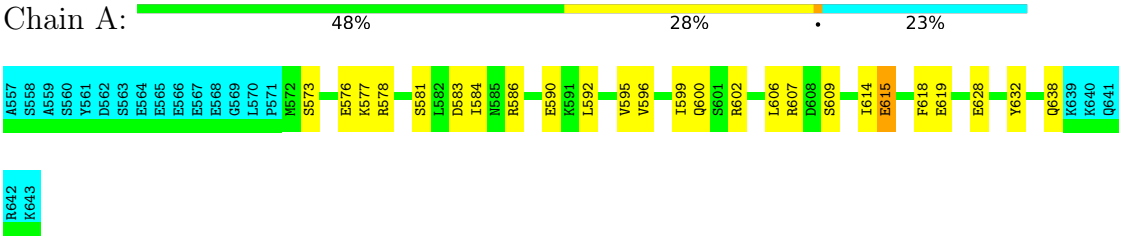
• Molecule 2: Brd3_ET

Chain B:

4.2.16 Score per residue for model 16

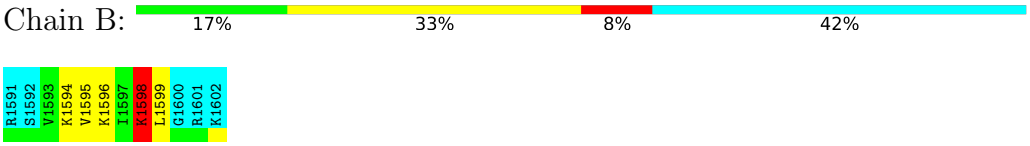
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

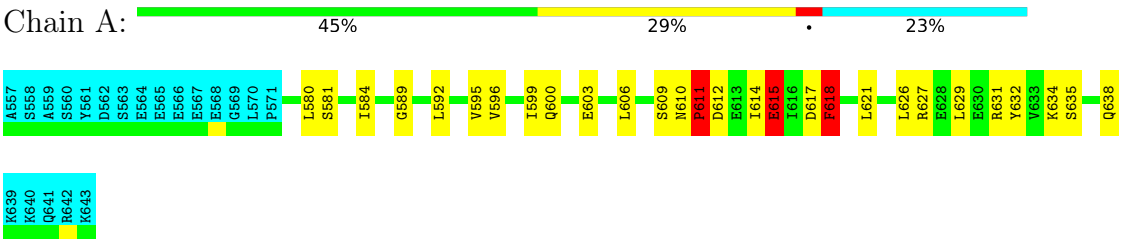
Chain B:



4.2.17 Score per residue for model 17

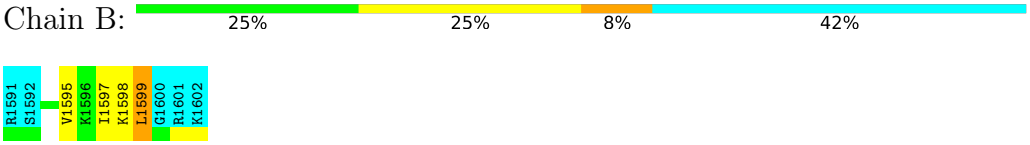
• Molecule 1: Bromodomain-containing protein 3

Chain A:



• Molecule 2: Brd3_ET

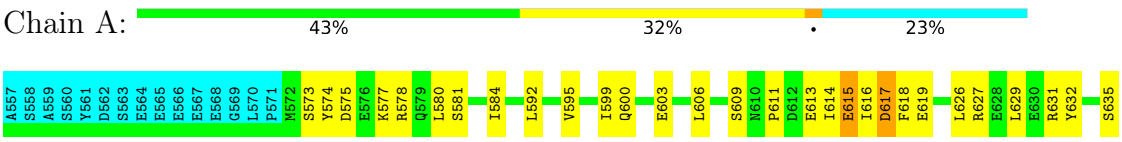
Chain B:

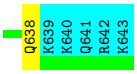


4.2.18 Score per residue for model 18

• Molecule 1: Bromodomain-containing protein 3

Chain A:





• Molecule 2: Brd3_ET

Chain B:

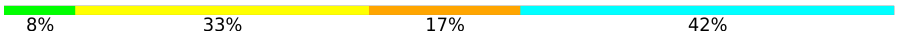
4.2.19 Score per residue for model 19

• Molecule 1: Bromodomain-containing protein 3

Chain A:

• Molecule 2: Brd3_ET

Chain B:



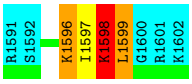
4.2.20 Score per residue for model 20

• Molecule 1: Bromodomain-containing protein 3

Chain A:

• Molecule 2: Brd3_ET

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 20 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	

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	1102
Number of shifts mapped to atoms	1102
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality

6.1 Standard geometry

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	0.78±0.04	0±0/561 (0.0± 0.1%)	0.83±0.06	0±0/756 (0.1± 0.1%)
2	B	0.82±0.07	0±0/57 (0.0± 0.0%)	0.85±0.10	0±0/75 (0.0± 0.0%)
All	All	0.79	2/12360 (0.0%)	0.83	8/16620 (0.0%)

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	0.4±0.8
All	All	0	8

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	615	GLU	CD-OE2	-5.91	1.19	1.25	17	1
1	A	611	PRO	N-CD	-5.06	1.40	1.47	5	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	611	PRO	N-CD-CG	-6.49	93.47	103.20	11	2
1	A	611	PRO	CA-N-CD	-6.15	102.89	111.50	17	1
1	A	615	GLU	CA-CB-CG	5.47	125.44	113.40	19	5

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	631	ARG	Sidechain	3
1	A	602	ARG	Sidechain	1
1	A	607	ARG	Sidechain	1
1	A	627	ARG	Sidechain	1
1	A	586	ARG	Sidechain	1
1	A	578	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	553	561	561	18±3
2	B	57	79	79	10±2
All	All	12200	12800	12800	387

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:581:SER:HB2	2:B:1595:VAL:HG13	0.79	1.52	18	16
1:A:616:ILE:O	2:B:1596:LYS:HA	0.74	1.81	5	14
1:A:577:LYS:HD3	1:A:618:PHE:O	0.69	1.87	1	5
1:A:600:GLN:O	1:A:605:SER:HA	0.66	1.90	10	1
1:A:596:VAL:O	1:A:600:GLN:HB2	0.65	1.91	14	8
1:A:615:GLU:HG2	2:B:1598:LYS:HE2	0.65	1.66	6	5
1:A:615:GLU:HG3	2:B:1598:LYS:HE3	0.64	1.67	17	4
1:A:589:GLY:HA2	1:A:592:LEU:HD23	0.64	1.69	17	5
1:A:596:VAL:O	1:A:600:GLN:HG3	0.63	1.93	5	2
1:A:592:LEU:HD22	2:B:1599:LEU:HG	0.62	1.72	2	19
1:A:615:GLU:HB3	2:B:1598:LYS:HD2	0.62	1.72	4	5
1:A:572:MET:SD	1:A:623:PRO:HG3	0.62	2.34	19	2
1:A:615:GLU:HB2	2:B:1598:LYS:HD3	0.60	1.73	13	10
1:A:627:ARG:O	1:A:631:ARG:HG3	0.60	1.97	4	9
1:A:635:SER:O	1:A:638:GLN:HG2	0.60	1.96	17	5
1:A:600:GLN:HB3	1:A:606:LEU:HD22	0.59	1.75	1	1
1:A:615:GLU:HB3	2:B:1598:LYS:HD3	0.59	1.72	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:595:VAL:O	1:A:599:ILE:HG12	0.59	1.98	12	20
1:A:609:SER:O	1:A:611:PRO:HD3	0.59	1.98	11	2
1:A:615:GLU:HG2	2:B:1598:LYS:HE3	0.58	1.74	14	2
1:A:615:GLU:HG3	2:B:1598:LYS:HE2	0.58	1.74	5	3
1:A:616:ILE:HB	2:B:1597:ILE:HB	0.58	1.74	15	2
1:A:618:PHE:CE2	1:A:626:LEU:HA	0.58	2.33	17	1
1:A:589:GLY:O	1:A:592:LEU:HG	0.58	1.98	20	7
1:A:578:ARG:HB2	2:B:1595:VAL:HG22	0.57	1.76	8	5
1:A:615:GLU:HA	2:B:1597:ILE:HG22	0.57	1.76	6	2
1:A:627:ARG:O	1:A:631:ARG:HG2	0.56	1.99	18	3
1:A:610:ASN:HB3	1:A:611:PRO:HD2	0.56	1.77	17	1
1:A:604:PRO:O	1:A:609:SER:HA	0.56	2.01	7	1
1:A:607:ARG:NE	1:A:607:ARG:HA	0.56	2.16	5	1
1:A:614:ILE:O	2:B:1598:LYS:HA	0.55	2.02	4	8
1:A:600:GLN:OE1	1:A:607:ARG:HB3	0.55	2.02	1	1
1:A:619:GLU:CD	2:B:1594:LYS:HA	0.55	2.22	11	8
1:A:606:LEU:HD12	1:A:607:ARG:H	0.54	1.62	1	1
1:A:592:LEU:HD22	2:B:1599:LEU:CG	0.53	2.33	17	19
2:B:1597:ILE:HD12	2:B:1599:LEU:HD22	0.53	1.80	3	1
1:A:615:GLU:CG	2:B:1598:LYS:HE2	0.53	2.34	6	1
1:A:607:ARG:HA	1:A:607:ARG:NE	0.52	2.20	12	2
1:A:618:PHE:CZ	1:A:626:LEU:HA	0.52	2.38	6	3
1:A:581:SER:HB2	2:B:1595:VAL:CG1	0.52	2.33	10	3
1:A:595:VAL:HB	1:A:632:TYR:CZ	0.52	2.40	18	7
1:A:582:LEU:O	1:A:586:ARG:HG2	0.52	2.04	4	2
1:A:581:SER:HB3	2:B:1595:VAL:CG1	0.52	2.35	7	1
1:A:619:GLU:HG3	2:B:1594:LYS:HA	0.52	1.81	8	1
2:B:1597:ILE:HG23	2:B:1598:LYS:N	0.51	2.20	7	16
1:A:616:ILE:H	2:B:1597:ILE:HG22	0.51	1.65	6	2
1:A:592:LEU:HD22	2:B:1599:LEU:HB3	0.51	1.83	16	5
1:A:615:GLU:HA	2:B:1597:ILE:O	0.51	2.05	18	2
1:A:600:GLN:O	1:A:607:ARG:HD2	0.51	2.05	15	2
1:A:584:ILE:HG13	2:B:1599:LEU:HD21	0.51	1.81	4	4
1:A:615:GLU:HG2	2:B:1598:LYS:CE	0.50	2.36	14	2
1:A:615:GLU:HG3	2:B:1598:LYS:CE	0.50	2.37	8	2
1:A:616:ILE:HD13	2:B:1597:ILE:HG21	0.49	1.83	6	2
1:A:578:ARG:HB2	2:B:1595:VAL:CG2	0.49	2.36	8	1
1:A:615:GLU:HB3	2:B:1598:LYS:HE2	0.49	1.83	1	1
1:A:629:LEU:O	1:A:633:VAL:HG23	0.49	2.07	6	7
1:A:581:SER:CB	2:B:1595:VAL:HG13	0.49	2.38	2	6
1:A:596:VAL:CG2	1:A:614:ILE:HB	0.49	2.37	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:633:VAL:O	1:A:637:LEU:HG	0.49	2.08	9	4
1:A:589:GLY:HA2	1:A:592:LEU:CD2	0.48	2.38	11	6
1:A:618:PHE:HA	1:A:621:LEU:HB3	0.48	1.84	20	4
1:A:617:ASP:HA	2:B:1596:LYS:HD2	0.48	1.85	18	2
1:A:619:GLU:HG3	2:B:1595:VAL:H	0.47	1.68	2	3
1:A:580:LEU:O	1:A:584:ILE:HG22	0.47	2.08	18	5
1:A:607:ARG:HD2	1:A:610:ASN:O	0.47	2.09	1	1
1:A:606:LEU:HD23	1:A:607:ARG:HG2	0.47	1.85	5	1
1:A:584:ILE:HG23	2:B:1597:ILE:HG13	0.47	1.85	15	2
1:A:616:ILE:N	2:B:1597:ILE:HG22	0.47	2.24	6	3
1:A:574:TYR:O	1:A:578:ARG:HB2	0.47	2.09	18	2
1:A:588:PRO:HG2	1:A:591:LYS:HD3	0.46	1.86	5	1
1:A:592:LEU:HD12	1:A:593:GLY:N	0.46	2.25	5	1
1:A:603:GLU:O	1:A:606:LEU:HD23	0.46	2.10	18	1
1:A:572:MET:HA	1:A:576:GLU:OE1	0.46	2.10	1	1
1:A:573:SER:O	1:A:577:LYS:HG2	0.46	2.11	16	2
1:A:581:SER:HB3	2:B:1595:VAL:HG13	0.46	1.85	7	1
1:A:634:LYS:O	1:A:638:GLN:HG3	0.46	2.10	2	1
1:A:607:ARG:O	1:A:617:ASP:HB2	0.46	2.11	1	1
1:A:584:ILE:HD13	1:A:595:VAL:HG11	0.45	1.88	20	3
1:A:576:GLU:O	1:A:579:GLN:HG2	0.45	2.11	12	1
1:A:630:GLU:O	1:A:634:LYS:HG2	0.45	2.12	8	1
1:A:602:ARG:HD2	1:A:628:GLU:OE1	0.45	2.11	14	3
1:A:600:GLN:HG2	1:A:606:LEU:HD22	0.45	1.87	5	1
1:A:602:ARG:HD2	1:A:628:GLU:OE2	0.45	2.12	6	2
1:A:582:LEU:O	1:A:586:ARG:HG3	0.45	2.11	14	1
1:A:616:ILE:H	2:B:1597:ILE:H	0.45	1.54	9	2
1:A:602:ARG:HB2	1:A:625:THR:HG23	0.45	1.89	20	1
1:A:610:ASN:CB	1:A:611:PRO:HD2	0.45	2.42	17	1
1:A:610:ASN:HB3	1:A:611:PRO:CD	0.45	2.41	17	1
1:A:618:PHE:HB2	2:B:1595:VAL:CG1	0.44	2.41	6	2
1:A:600:GLN:HG3	1:A:606:LEU:HB3	0.44	1.88	12	1
1:A:578:ARG:CZ	2:B:1593:VAL:HA	0.44	2.42	12	1
1:A:582:LEU:O	1:A:586:ARG:HB2	0.44	2.13	7	1
1:A:623:PRO:O	1:A:626:LEU:HB3	0.44	2.13	1	2
1:A:586:ARG:HA	1:A:586:ARG:NE	0.43	2.28	3	1
1:A:584:ILE:O	2:B:1599:LEU:HD21	0.43	2.13	13	1
1:A:578:ARG:HD2	2:B:1594:LYS:O	0.43	2.13	19	2
1:A:623:PRO:O	1:A:627:ARG:HG3	0.43	2.13	1	1
1:A:596:VAL:HG21	1:A:614:ILE:HA	0.43	1.90	3	1
1:A:591:LYS:HG2	1:A:636:CYS:SG	0.43	2.53	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:580:LEU:HB3	1:A:629:LEU:HD23	0.43	1.89	18	1
1:A:573:SER:O	1:A:577:LYS:HG3	0.42	2.14	9	3
1:A:578:ARG:CB	2:B:1595:VAL:HG22	0.42	2.44	13	1
1:A:619:GLU:OE1	2:B:1594:LYS:HG3	0.42	2.14	12	1
1:A:616:ILE:HD13	2:B:1597:ILE:CG2	0.42	2.44	20	1
1:A:584:ILE:HG13	2:B:1599:LEU:CD2	0.42	2.45	14	3
1:A:590:GLU:O	1:A:594:ARG:HG3	0.42	2.14	10	1
1:A:591:LYS:O	1:A:595:VAL:HG23	0.42	2.15	14	2
1:A:592:LEU:HD13	1:A:614:ILE:HG21	0.42	1.92	8	2
1:A:610:ASN:ND2	1:A:612:ASP:HB3	0.42	2.30	8	1
1:A:592:LEU:CB	2:B:1599:LEU:HG	0.42	2.44	9	1
1:A:577:LYS:HG2	1:A:626:LEU:HD12	0.42	1.92	18	1
1:A:591:LYS:HD3	1:A:636:CYS:SG	0.42	2.54	4	1
1:A:627:ARG:HD2	1:A:627:ARG:O	0.41	2.14	8	1
1:A:600:GLN:HG2	1:A:606:LEU:HB3	0.41	1.92	5	1
1:A:638:GLN:O	1:A:638:GLN:HG3	0.41	2.15	19	1
1:A:634:LYS:O	1:A:638:GLN:HG2	0.41	2.16	4	1
1:A:590:GLU:HG3	1:A:591:LYS:HD2	0.41	1.91	5	1
1:A:603:GLU:OE2	1:A:604:PRO:HD2	0.41	2.15	10	1
1:A:603:GLU:O	1:A:607:ARG:HG3	0.41	2.15	3	1
1:A:592:LEU:HD22	2:B:1599:LEU:CB	0.41	2.46	16	1
1:A:603:GLU:HG3	1:A:621:LEU:HD11	0.41	1.92	17	1
1:A:592:LEU:CD2	2:B:1599:LEU:HG	0.41	2.44	2	1
1:A:623:PRO:HA	1:A:626:LEU:HB3	0.41	1.92	8	1
1:A:600:GLN:HA	1:A:603:GLU:OE1	0.41	2.16	15	1
1:A:614:ILE:HD13	2:B:1599:LEU:HB2	0.41	1.92	2	1
1:A:610:ASN:O	1:A:612:ASP:N	0.41	2.53	17	1
2:B:1597:ILE:CG2	2:B:1598:LYS:N	0.40	2.84	7	2
1:A:630:GLU:O	1:A:634:LYS:HG3	0.40	2.17	6	1
1:A:610:ASN:O	1:A:610:ASN:ND2	0.40	2.55	11	1
1:A:573:SER:O	1:A:576:GLU:HB3	0.40	2.17	16	1
1:A:592:LEU:O	1:A:614:ILE:HD12	0.40	2.15	18	1
1:A:617:ASP:O	1:A:619:GLU:N	0.40	2.53	18	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	67/87 (77%)	62±3 (92±4%)	3±1 (5±2%)	2±2 (3±3%)	8 44
2	B	7/12 (58%)	3±1 (43±12%)	3±1 (46±12%)	1±1 (11±11%)	1 8
All	All	1480/1980 (75%)	1299 (88%)	130 (9%)	51 (3%)	6 36

All 13 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	618	PHE	10
1	A	609	SER	7
2	B	1596	LYS	6
2	B	1598	LYS	5
1	A	606	LEU	5
1	A	617	ASP	5
2	B	1597	ILE	4
1	A	611	PRO	3
1	A	613	GLU	2
1	A	604	PRO	1
2	B	1594	LYS	1
1	A	638	GLN	1
1	A	605	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	65/82 (79%)	60±2 (93±3%)	5±2 (7±3%)	17 65
2	B	7/11 (64%)	6±1 (81±8%)	1±1 (19±8%)	4 35
All	All	1440/1860 (77%)	1316 (91%)	124 (9%)	14 61

All 32 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	615	GLU	19

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Mol	Chain	Res	Type	Models (Total)
2	B	1599	LEU	15
1	A	629	LEU	9
1	A	606	LEU	8
1	A	578	ARG	8
1	A	620	THR	7
2	B	1598	LYS	6
1	A	590	GLU	6
1	A	603	GLU	6
2	B	1597	ILE	3
1	A	618	PHE	3
1	A	625	THR	3
1	A	630	GLU	3
1	A	638	GLN	3
1	A	575	ASP	2
1	A	600	GLN	2
2	B	1596	LYS	2
1	A	583	ASP	2
1	A	596	VAL	2
1	A	572	MET	2
1	A	631	ARG	2
1	A	604	PRO	1
1	A	617	ASP	1
2	B	1595	VAL	1
1	A	602	ARG	1
1	A	634	LYS	1
1	A	622	LYS	1
1	A	610	ASN	1
1	A	581	SER	1
1	A	591	LYS	1
1	A	586	ARG	1
1	A	613	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

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *testv21.str*

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	1102
Number of shifts mapped to atoms	1102
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	86	-0.51 ± 0.19	Should be applied
$^{13}C_{\beta}$	83	-0.11 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	79	0.30 ± 0.16	None needed (< 0.5 ppm)
^{15}N	77	-0.07 ± 0.23	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 79%, i.e. 786 atoms were assigned a chemical shift out of a possible 994. 11 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	332/362 (92%)	142/144 (99%)	129/148 (87%)	61/70 (87%)
Sidechain	442/600 (74%)	287/353 (81%)	152/214 (71%)	3/33 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	12/32 (38%)	12/17 (71%)	0/14 (0%)	0/1 (0%)
Overall	786/994 (79%)	441/514 (86%)	281/376 (75%)	64/104 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 995 atoms were assigned a chemical shift out of a possible 1317. 12 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	427/485 (88%)	185/193 (96%)	165/198 (83%)	77/94 (82%)
Sidechain	552/792 (70%)	365/469 (78%)	184/276 (67%)	3/47 (6%)
Aromatic	16/40 (40%)	16/21 (76%)	0/18 (0%)	0/1 (0%)
Overall	995/1317 (76%)	566/683 (83%)	349/492 (71%)	80/142 (56%)

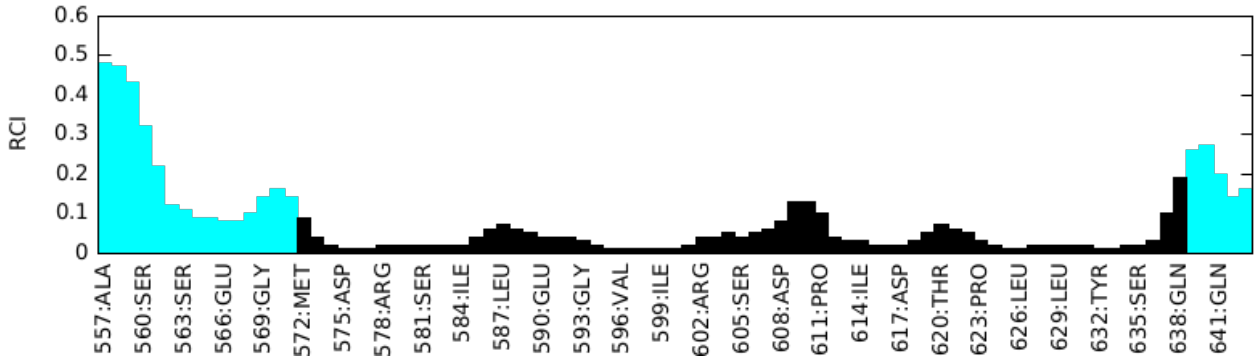
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

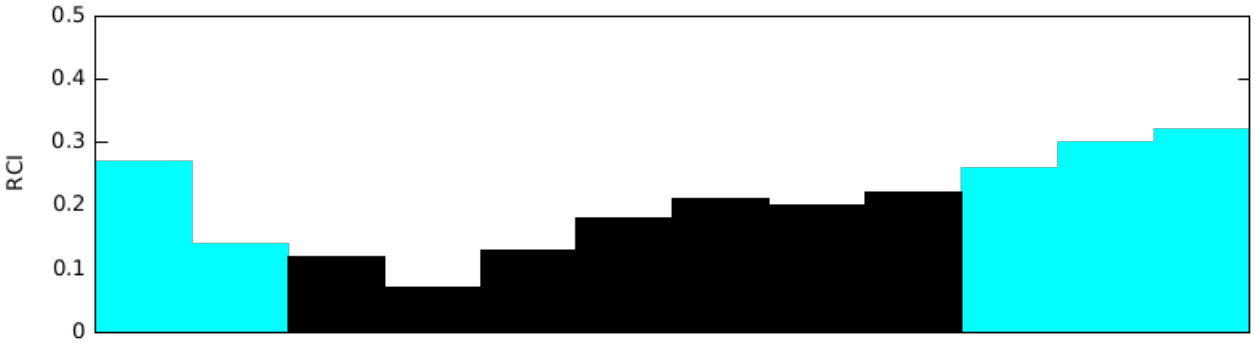
7.1.5 Random Coil Index (RCI) plots (i)

The images below report *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:



Random coil index (RCI) for chain B:


RCI
0.5
0.4
0.3
0.2
0.1
0