



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:55 AM BST

PDB ID : 5IAY
Title : NMR structure of UHRF1 Tandem Tudor Domains in a complex with Spacer peptide
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Deposited on : 2016-02-22

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

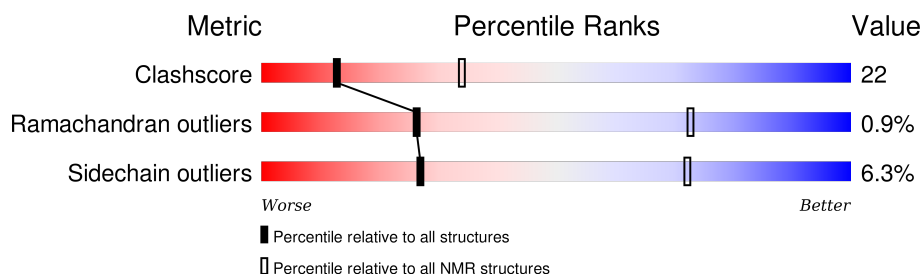
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 64%.

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	152	
2	B	16	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:135-A:160, A:182-A:282, B:648-B:653 (133)	0.30	19

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2697 atoms, of which 1332 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms						Trace
1	A	152	Total	C	H	N	O	S	0
			2463	779	1211	225	243	5	

- Molecule 2 is a protein called Spacer.

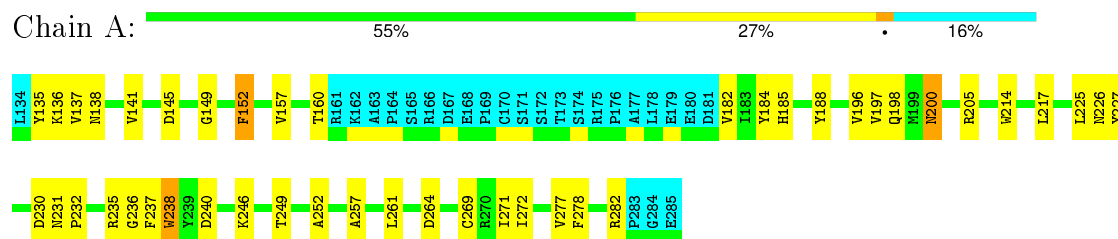
Mol	Chain	Residues	Atoms					Trace
2	B	16	Total	C	H	N	O	0
			234	69	121	24	20	

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: E3 ubiquitin-protein ligase UHRF1



- Molecule 2: Spacer

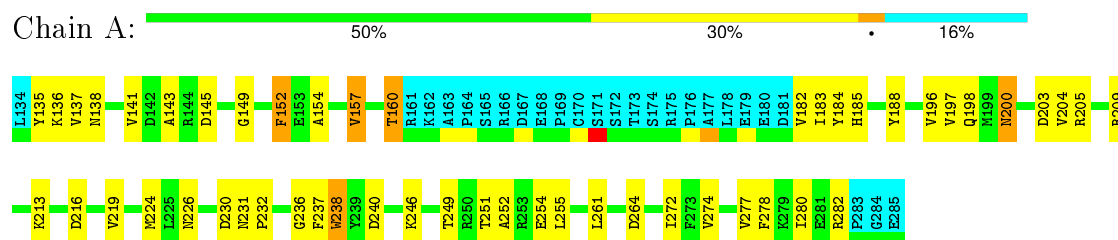


4.2 Scores per residue for each member of the ensemble

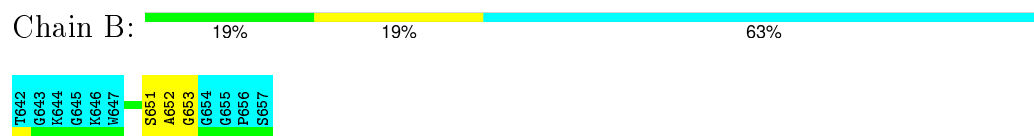
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

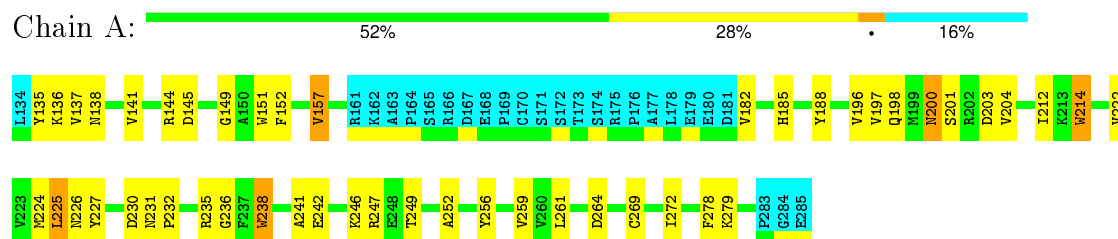


- Molecule 2: Spacer

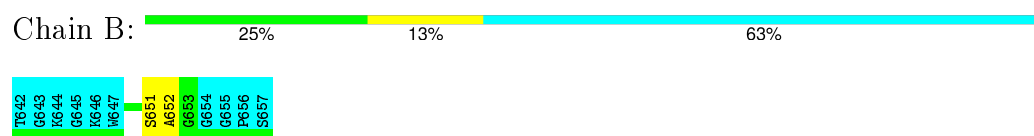


4.2.2 Score per residue for model 2

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

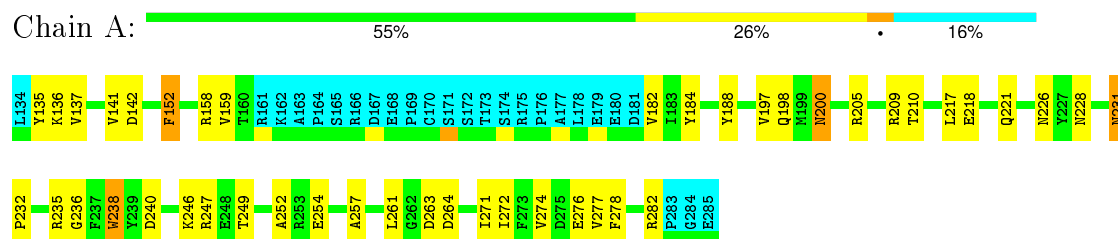


- Molecule 2: Spacer

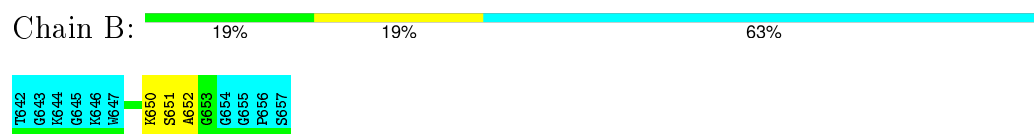


4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

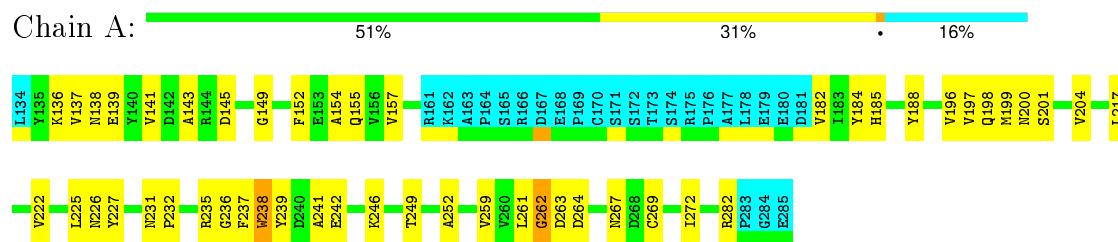


- Molecule 2: Spacer

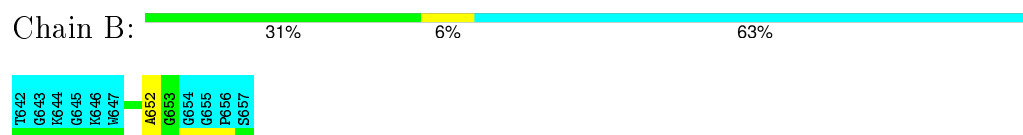


4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

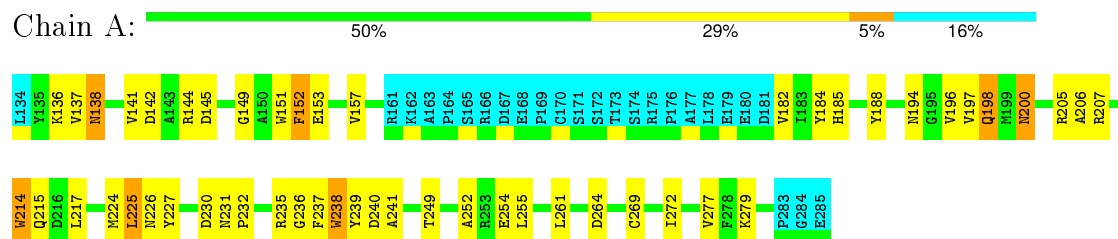


- Molecule 2: Spacer



4.2.5 Score per residue for model 5

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

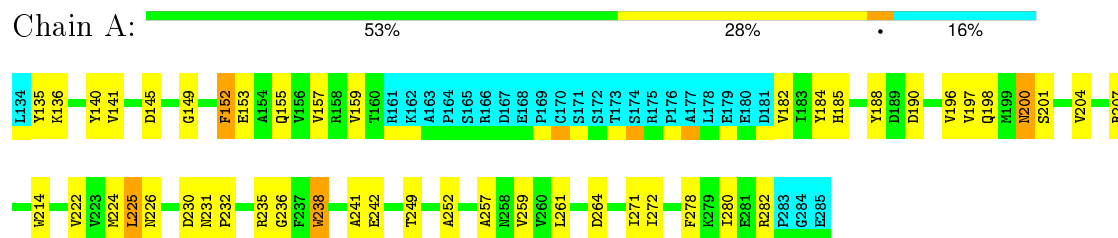


- Molecule 2: Spacer

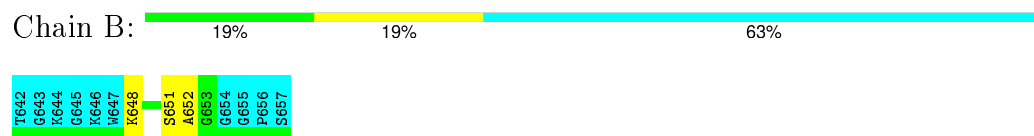


4.2.6 Score per residue for model 6

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

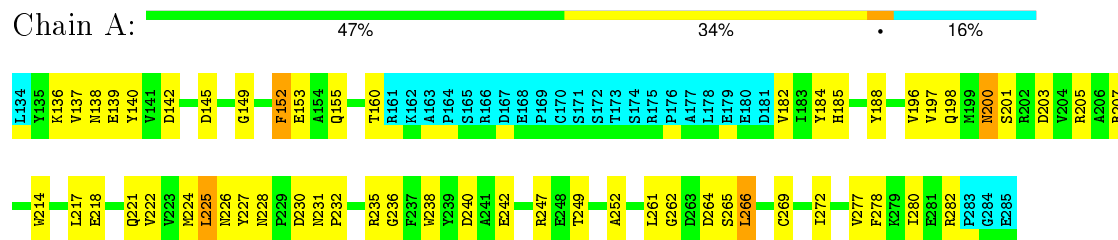


- Molecule 2: Spacer

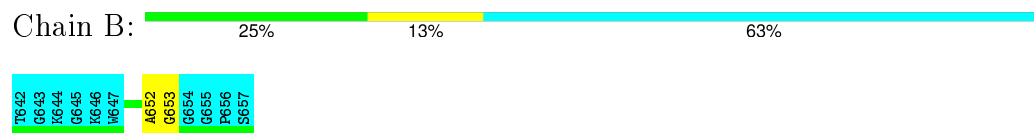


4.2.7 Score per residue for model 7

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

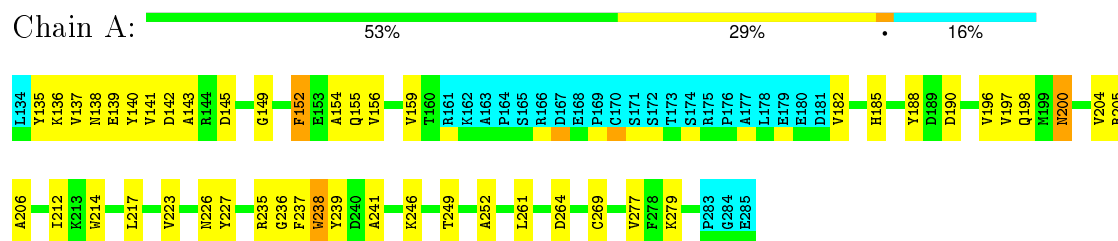


- Molecule 2: Spacer



4.2.8 Score per residue for model 8

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

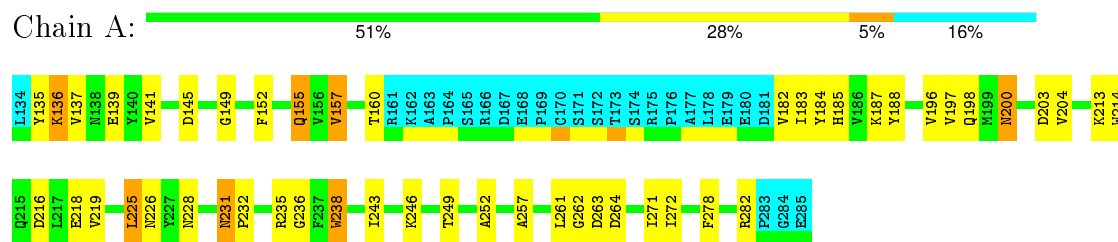


- Molecule 2: Spacer

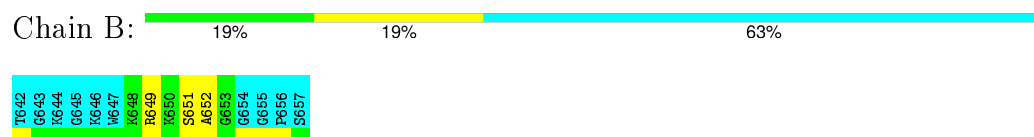


4.2.9 Score per residue for model 9

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

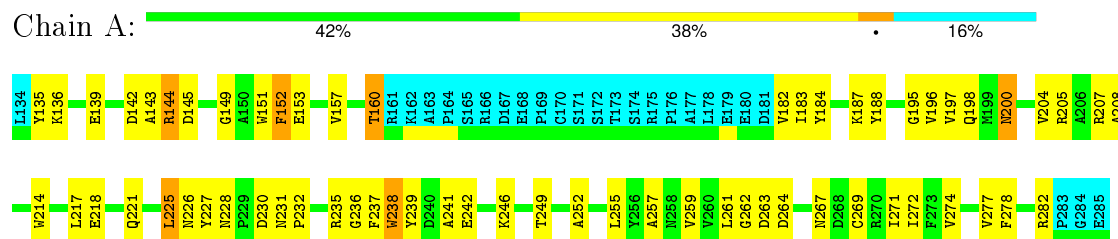


- Molecule 2: Spacer

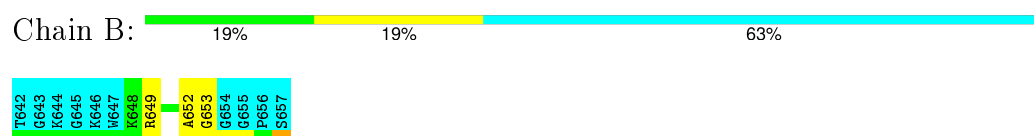


4.2.10 Score per residue for model 10

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

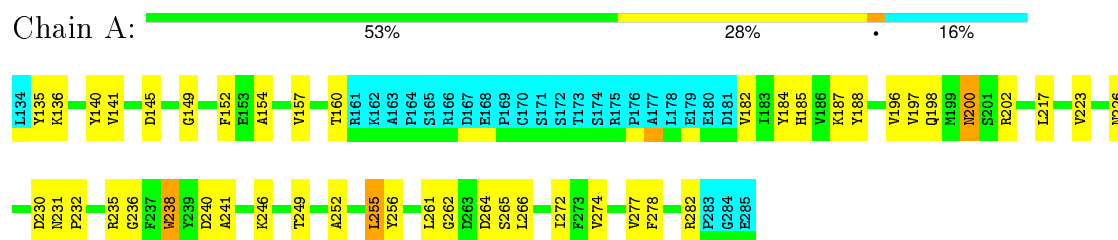


- Molecule 2: Spacer

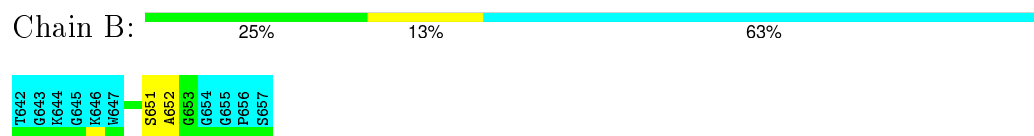


4.2.11 Score per residue for model 11

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

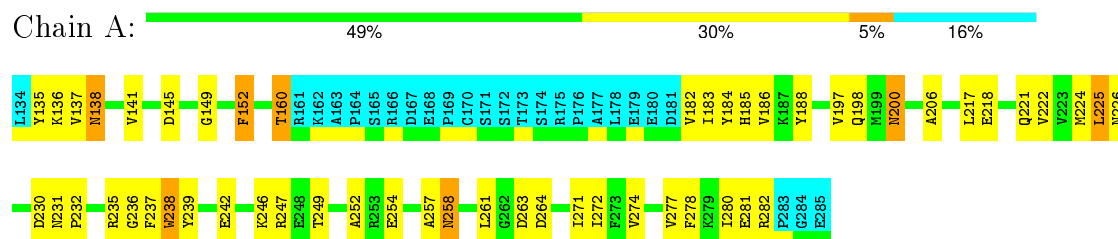


- Molecule 2: Spacer

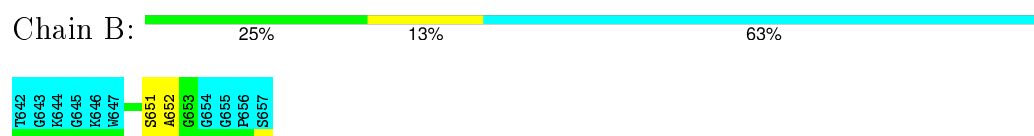


4.2.12 Score per residue for model 12

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

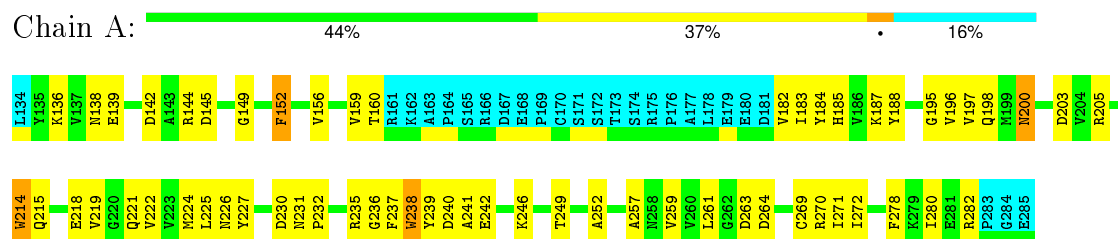


- Molecule 2: Spacer



4.2.13 Score per residue for model 13

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

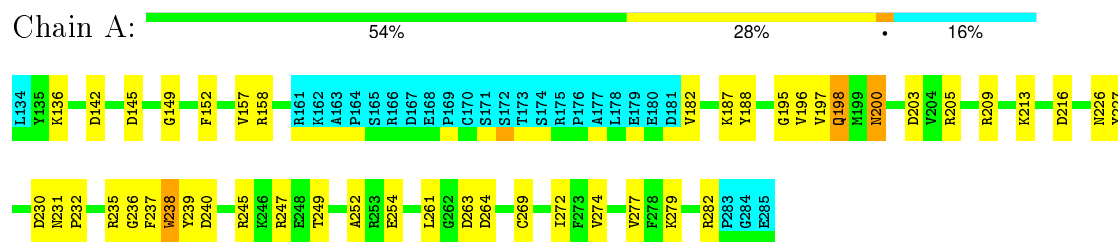


- Molecule 2: Spacer

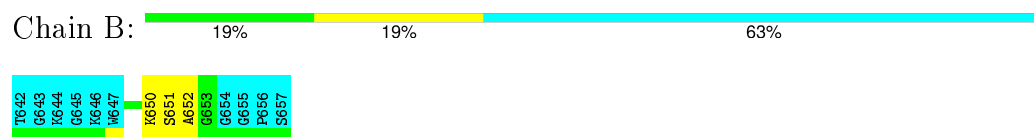


4.2.14 Score per residue for model 14

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

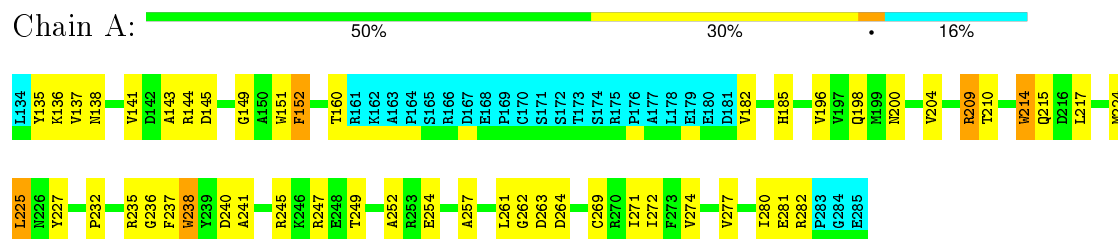


- Molecule 2: Spacer

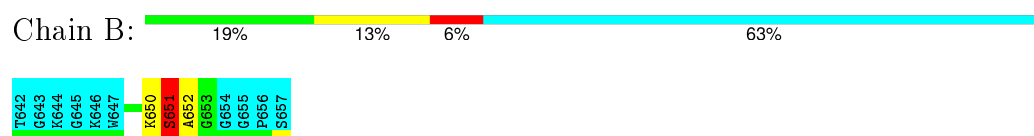


4.2.15 Score per residue for model 15

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

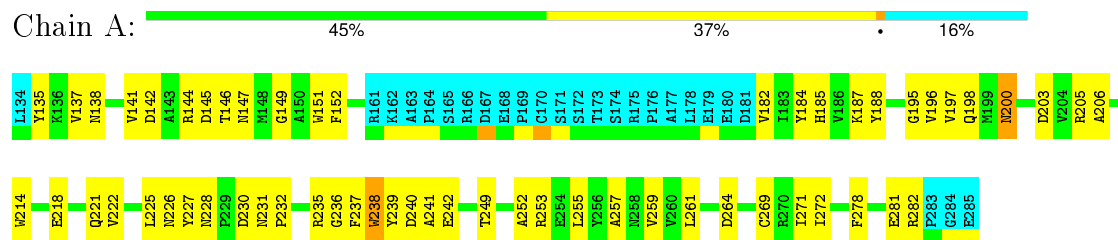


- Molecule 2: Spacer

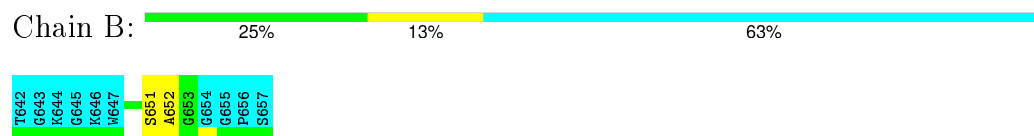


4.2.16 Score per residue for model 16

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

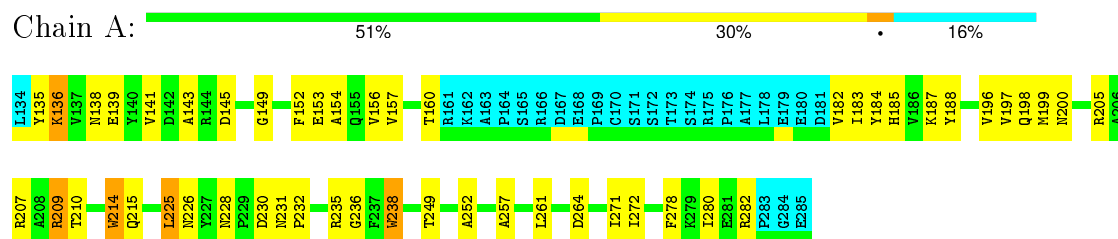


- Molecule 2: Spacer



4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

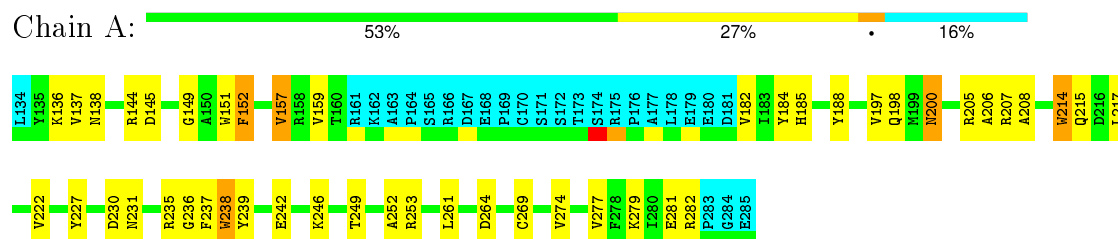


- Molecule 2: Spacer

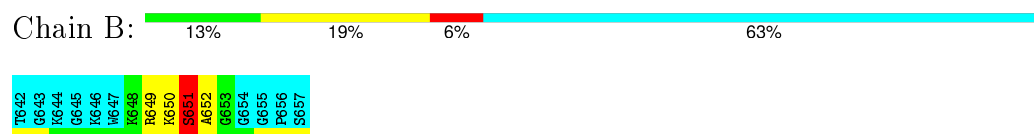


4.2.18 Score per residue for model 18

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

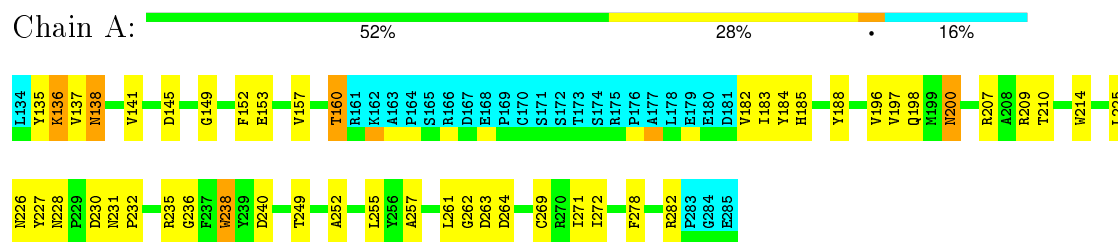


- Molecule 2: Spacer

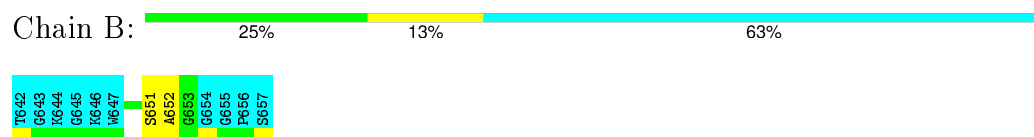


4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

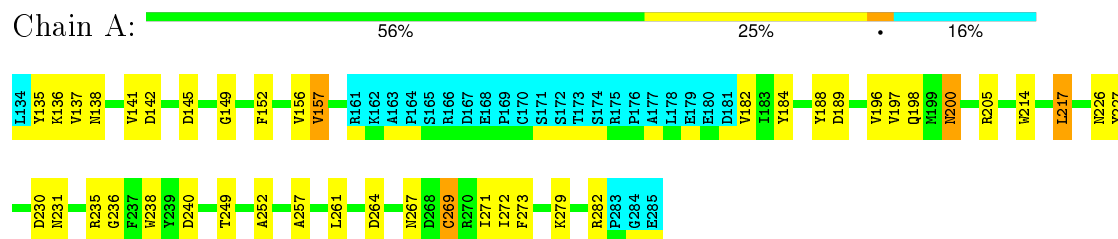


- Molecule 2: Spacer

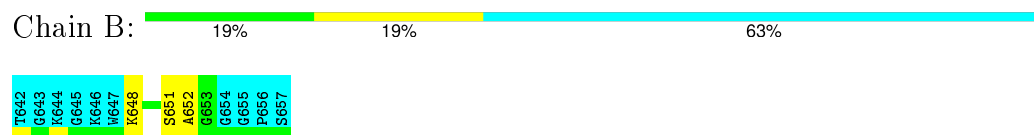


4.2.20 Score per residue for model 20

- Molecule 1: E3 ubiquitin-protein ligase UHRF1



- Molecule 2: Spacer



5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR 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)	5iay_cs.str
Number of chemical shift lists	1
Total number of shifts	1464
Number of shifts mapped to atoms	1464
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1062	1030	1029	47±5
2	B	44	52	52	5±2
All	All	22120	21640	21620	949

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:225:LEU:HD23	1:A:225:LEU:N	0.84	1.88	5	5
1:A:225:LEU:N	1:A:225:LEU:HD23	0.84	1.87	2	3
1:A:188:TYR:CZ	1:A:197:VAL:HG21	0.83	2.08	6	14
1:A:224:MET:SD	1:A:280:ILE:HD11	0.83	2.13	1	1
1:A:225:LEU:HD21	1:A:241:ALA:HB3	0.82	1.51	5	4
1:A:188:TYR:OH	1:A:197:VAL:HG11	0.82	1.74	9	11
1:A:265:SER:O	1:A:266:LEU:HD12	0.77	1.79	11	1
1:A:135:TYR:CD1	1:A:141:VAL:HG11	0.72	2.19	20	7
1:A:265:SER:O	1:A:266:LEU:HD22	0.72	1.85	7	1
1:A:249:THR:OG1	1:A:252:ALA:HB3	0.71	1.86	12	20
1:A:226:ASN:ND2	1:A:238:TRP:CD2	0.69	2.60	4	2
1:A:188:TYR:CE2	1:A:197:VAL:HG21	0.69	2.22	9	5
1:A:214:TRP:CD1	1:A:215:GLN:N	0.69	2.61	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:214:TRP:CE3	1:A:253:ARG:NH2	0.69	2.61	16	1
1:A:238:TRP:CH2	1:A:278:PHE:CD2	0.69	2.80	1	4
1:A:225:LEU:HD23	1:A:225:LEU:O	0.68	1.88	17	1
1:A:152:PHE:N	1:A:152:PHE:CD1	0.67	2.62	18	1
1:A:137:VAL:HG13	1:A:157:VAL:O	0.67	1.90	20	6
1:A:232:PRO:O	1:A:272:ILE:HD12	0.67	1.89	2	17
1:A:227:TYR:CE1	1:A:269:CYS:SG	0.67	2.88	2	10
1:A:227:TYR:CZ	1:A:269:CYS:SG	0.66	2.88	2	3
1:A:196:VAL:HG12	1:A:198:GLN:HE22	0.65	1.52	4	3
1:A:144:ARG:NE	1:A:151:TRP:CZ2	0.65	2.65	16	6
1:A:137:VAL:HG12	1:A:138:ASN:ND2	0.64	2.08	15	2
1:A:225:LEU:HD23	1:A:225:LEU:C	0.64	2.13	17	1
1:A:225:LEU:N	1:A:225:LEU:CD2	0.63	2.60	2	3
1:A:225:LEU:CD2	1:A:225:LEU:N	0.63	2.60	5	3
1:A:136:LYS:CB	1:A:136:LYS:NZ	0.63	2.61	17	1
1:A:144:ARG:NH1	1:A:151:TRP:HE1	0.63	1.92	15	1
1:A:137:VAL:O	1:A:138:ASN:ND2	0.62	2.32	12	4
1:A:188:TYR:OH	1:A:197:VAL:HG21	0.62	1.95	13	9
1:A:224:MET:C	1:A:225:LEU:HD23	0.62	2.14	15	5
1:A:253:ARG:NH2	1:A:255:LEU:HD21	0.62	2.09	16	1
1:A:196:VAL:HG22	1:A:198:GLN:HE22	0.62	1.53	7	7
1:A:249:THR:OG1	1:A:252:ALA:N	0.62	2.33	10	20
1:A:217:LEU:HD12	1:A:217:LEU:O	0.62	1.94	20	1
1:A:236:GLY:N	2:B:652:ALA:O	0.61	2.33	18	20
1:A:185:HIS:ND1	1:A:198:GLN:OE1	0.61	2.34	6	7
1:A:185:HIS:CD2	1:A:198:GLN:OE1	0.61	2.54	18	10
1:A:153:GLU:OE2	2:B:649:ARG:N	0.61	2.34	17	1
1:A:145:ASP:O	1:A:149:GLY:N	0.61	2.34	2	19
1:A:198:GLN:H	1:A:198:GLN:NE2	0.60	1.93	14	1
1:A:185:HIS:CE1	1:A:198:GLN:OE1	0.60	2.55	1	6
1:A:226:ASN:OD1	1:A:238:TRP:CD2	0.60	2.54	5	11
1:A:245:ARG:NH2	1:A:247:ARG:HH11	0.60	1.94	14	1
1:A:185:HIS:ND1	1:A:198:GLN:NE2	0.60	2.49	12	3
1:A:137:VAL:CG2	1:A:159:VAL:HG12	0.60	2.26	8	1
1:A:159:VAL:HG13	1:A:159:VAL:O	0.60	1.97	18	1
1:A:219:VAL:CG2	1:A:246:LYS:HZ2	0.60	2.10	1	2
1:A:185:HIS:CG	1:A:198:GLN:OE1	0.60	2.55	15	13
1:A:196:VAL:O	1:A:198:GLN:NE2	0.60	2.35	5	10
1:A:214:TRP:CZ3	1:A:255:LEU:HD21	0.60	2.32	10	2
1:A:247:ARG:HH22	1:A:249:THR:HG22	0.59	1.55	7	2
1:A:159:VAL:O	1:A:159:VAL:HG13	0.59	1.97	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:ARG:CZ	1:A:151:TRP:HE1	0.59	2.10	15	1
1:A:146:THR:HG23	1:A:147:ASN:ND2	0.59	2.11	16	1
1:A:263:ASP:OD1	1:A:264:ASP:N	0.59	2.36	12	3
1:A:226:ASN:OD1	1:A:238:TRP:CD1	0.59	2.56	17	4
1:A:228:ASN:ND2	1:A:231:ASN:OD1	0.59	2.36	3	2
1:A:226:ASN:OD1	1:A:238:TRP:CE3	0.59	2.56	20	3
1:A:144:ARG:CZ	1:A:151:TRP:NE1	0.59	2.65	15	1
1:A:144:ARG:NH1	1:A:240:ASP:OD2	0.59	2.35	15	1
1:A:214:TRP:O	1:A:217:LEU:HD11	0.59	1.98	20	1
1:A:231:ASN:OD1	1:A:231:ASN:N	0.59	2.35	3	1
1:A:140:TYR:CE1	1:A:155:GLN:NE2	0.59	2.70	8	2
1:A:237:PHE:O	1:A:239:TYR:CD2	0.59	2.56	13	9
1:A:238:TRP:CD1	2:B:651:SER:OG	0.59	2.56	16	8
1:A:217:LEU:O	1:A:246:LYS:NZ	0.59	2.35	18	7
1:A:226:ASN:OD1	1:A:238:TRP:CH2	0.59	2.56	4	1
1:A:272:ILE:CG2	1:A:273:PHE:CD2	0.58	2.86	20	1
1:A:235:ARG:CZ	2:B:652:ALA:CB	0.58	2.81	6	1
1:A:144:ARG:NH2	1:A:240:ASP:OD2	0.58	2.36	15	1
1:A:261:LEU:O	1:A:263:ASP:N	0.58	2.37	4	1
1:A:153:GLU:OE1	1:A:207:ARG:NH1	0.58	2.37	7	1
1:A:209:ARG:NH2	1:A:210:THR:OG1	0.58	2.36	15	2
1:A:190:ASP:OD1	2:B:648:LYS:NZ	0.58	2.37	8	2
1:A:187:LYS:NZ	1:A:195:GLY:O	0.58	2.36	16	3
1:A:140:TYR:CE1	1:A:155:GLN:OE1	0.58	2.57	7	1
1:A:140:TYR:CD1	1:A:155:GLN:OE1	0.58	2.56	7	1
1:A:184:TYR:CE1	1:A:201:SER:OG	0.58	2.56	7	1
1:A:228:ASN:ND2	2:B:653:GLY:O	0.58	2.36	7	2
1:A:200:ASN:OD1	1:A:202:ARG:NH1	0.58	2.36	11	1
1:A:238:TRP:CE2	2:B:651:SER:OG	0.58	2.51	18	1
1:A:238:TRP:NE1	2:B:651:SER:OG	0.58	2.37	2	11
1:A:153:GLU:OE2	1:A:207:ARG:NH1	0.58	2.36	6	3
1:A:139:GLU:O	1:A:155:GLN:NE2	0.58	2.36	7	3
1:A:209:ARG:NE	1:A:281:GLU:OE2	0.57	2.37	15	1
1:A:225:LEU:HD23	1:A:225:LEU:H	0.57	1.59	9	1
2:B:650:LYS:O	2:B:651:SER:CB	0.57	2.52	15	2
1:A:138:ASN:N	1:A:156:VAL:O	0.57	2.37	13	4
1:A:253:ARG:HH22	1:A:255:LEU:HD21	0.57	1.59	16	1
1:A:254:GLU:C	1:A:255:LEU:HD22	0.57	2.20	5	2
1:A:147:ASN:HD22	1:A:147:ASN:N	0.57	1.98	16	1
1:A:136:LYS:CB	1:A:136:LYS:HZ3	0.56	2.12	17	1
1:A:198:GLN:N	1:A:198:GLN:CD	0.56	2.58	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:LEU:CD2	1:A:277:VAL:HG11	0.56	2.30	15	4
1:A:153:GLU:OE1	2:B:649:ARG:N	0.56	2.38	5	1
1:A:227:TYR:OH	1:A:269:CYS:SG	0.56	2.64	20	3
1:A:198:GLN:CD	1:A:198:GLN:N	0.56	2.58	16	4
1:A:182:VAL:CG2	1:A:184:TYR:CZ	0.56	2.89	16	4
1:A:142:ASP:N	1:A:205:ARG:O	0.55	2.38	8	9
1:A:205:ARG:NH2	1:A:206:ALA:O	0.55	2.39	8	1
1:A:187:LYS:HE3	1:A:196:VAL:HG22	0.55	1.79	9	1
1:A:249:THR:OG1	1:A:252:ALA:CB	0.55	2.55	8	18
1:A:228:ASN:ND2	1:A:235:ARG:O	0.55	2.39	3	1
1:A:276:GLU:CD	2:B:650:LYS:HZ1	0.55	2.04	3	1
1:A:214:TRP:O	1:A:217:LEU:CD1	0.55	2.55	20	1
1:A:146:THR:HG23	1:A:147:ASN:HD22	0.55	1.60	16	1
1:A:137:VAL:O	1:A:138:ASN:CB	0.55	2.55	2	8
1:A:152:PHE:CE1	1:A:188:TYR:CD1	0.54	2.96	3	6
1:A:139:GLU:C	1:A:155:GLN:NE2	0.54	2.61	4	3
1:A:209:ARG:CD	1:A:209:ARG:N	0.54	2.71	15	1
1:A:197:VAL:C	1:A:198:GLN:NE2	0.54	2.61	8	8
1:A:238:TRP:CZ3	2:B:649:ARG:NH2	0.54	2.76	9	1
1:A:249:THR:HG1	1:A:252:ALA:C	0.54	2.04	11	9
1:A:276:GLU:CD	2:B:650:LYS:NZ	0.54	2.61	3	1
1:A:214:TRP:CE3	1:A:214:TRP:O	0.54	2.61	15	2
1:A:190:ASP:OD1	2:B:648:LYS:CE	0.54	2.56	8	1
1:A:208:ALA:H	2:B:649:ARG:HH12	0.54	1.44	10	1
1:A:188:TYR:OH	1:A:197:VAL:CG1	0.53	2.55	4	1
1:A:249:THR:OG1	1:A:252:ALA:CA	0.53	2.56	15	20
1:A:200:ASN:OD1	1:A:200:ASN:N	0.53	2.41	15	1
1:A:236:GLY:CA	2:B:652:ALA:O	0.53	2.57	4	11
1:A:222:VAL:HG22	1:A:242:GLU:HG2	0.53	1.81	7	8
1:A:160:THR:O	1:A:183:ILE:N	0.53	2.40	19	7
1:A:261:LEU:HD12	1:A:264:ASP:HB2	0.53	1.81	16	20
1:A:189:ASP:CG	2:B:648:LYS:NZ	0.53	2.62	20	1
1:A:257:ALA:HB3	1:A:271:ILE:HD11	0.52	1.81	15	8
1:A:243:ILE:HG21	1:A:246:LYS:NZ	0.52	2.20	9	1
1:A:219:VAL:CG2	1:A:246:LYS:NZ	0.52	2.73	1	1
1:A:196:VAL:C	1:A:198:GLN:NE2	0.52	2.62	17	9
1:A:235:ARG:HE	2:B:652:ALA:CB	0.52	2.17	4	1
1:A:196:VAL:C	1:A:198:GLN:HE22	0.52	2.08	17	5
1:A:143:ALA:HB1	1:A:199:MET:CE	0.52	2.35	4	2
1:A:253:ARG:HH11	1:A:274:VAL:CG2	0.51	2.17	18	1
1:A:214:TRP:C	1:A:214:TRP:CD1	0.51	2.82	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:214:TRP:C	1:A:214:TRP:CD2	0.51	2.80	15	2
1:A:240:ASP:OD1	1:A:240:ASP:O	0.51	2.28	11	5
1:A:240:ASP:O	1:A:240:ASP:OD1	0.51	2.28	13	3
1:A:136:LYS:NZ	1:A:138:ASN:HD21	0.51	2.03	19	1
1:A:205:ARG:NH2	1:A:240:ASP:OD2	0.51	2.43	5	2
1:A:187:LYS:CE	1:A:196:VAL:HG22	0.51	2.36	9	3
1:A:249:THR:HG1	1:A:252:ALA:H	0.51	1.47	20	7
1:A:241:ALA:HB2	1:A:259:VAL:HG22	0.51	1.83	13	6
1:A:238:TRP:CH2	1:A:278:PHE:CE2	0.51	2.99	17	4
1:A:238:TRP:CZ2	2:B:650:LYS:O	0.51	2.64	14	1
1:A:236:GLY:O	2:B:652:ALA:O	0.51	2.29	15	2
1:A:138:ASN:OD1	1:A:138:ASN:O	0.51	2.29	19	2
1:A:151:TRP:CZ2	1:A:240:ASP:OD2	0.51	2.64	5	1
1:A:200:ASN:OD1	1:A:202:ARG:CZ	0.50	2.58	11	1
1:A:138:ASN:O	1:A:138:ASN:OD1	0.50	2.29	12	1
1:A:247:ARG:NH2	1:A:249:THR:HG22	0.50	2.20	7	1
1:A:138:ASN:C	1:A:155:GLN:HE21	0.50	2.10	7	2
1:A:143:ALA:HB1	1:A:199:MET:HE1	0.50	1.82	17	2
1:A:144:ARG:NH1	1:A:205:ARG:NH1	0.50	2.60	18	1
1:A:201:SER:O	1:A:204:VAL:O	0.50	2.30	4	3
1:A:226:ASN:OD1	1:A:226:ASN:O	0.50	2.30	7	1
1:A:214:TRP:CD1	1:A:214:TRP:C	0.50	2.85	20	3
1:A:217:LEU:HD21	1:A:277:VAL:HG11	0.50	1.83	7	4
1:A:218:GLU:OE1	1:A:221:GLN:OE1	0.50	2.30	10	4
1:A:263:ASP:O	1:A:264:ASP:OD1	0.50	2.30	13	1
1:A:269:CYS:SG	1:A:270:ARG:N	0.50	2.84	13	1
1:A:186:VAL:O	1:A:197:VAL:HG22	0.50	2.07	12	1
1:A:247:ARG:O	1:A:254:GLU:O	0.49	2.30	12	4
1:A:144:ARG:NH1	1:A:203:ASP:OD1	0.49	2.44	13	1
1:A:249:THR:OG1	1:A:252:ALA:O	0.49	2.31	9	14
1:A:230:ASP:O	1:A:231:ASN:OD1	0.49	2.30	10	15
1:A:209:ARG:CD	1:A:209:ARG:H	0.49	2.20	15	1
1:A:196:VAL:HG13	1:A:196:VAL:O	0.49	2.07	1	3
1:A:141:VAL:O	1:A:154:ALA:O	0.49	2.31	4	5
1:A:198:GLN:N	1:A:198:GLN:NE2	0.49	2.60	14	1
1:A:212:ILE:HD11	1:A:279:LYS:HB3	0.49	1.82	2	1
1:A:218:GLU:OE2	1:A:221:GLN:OE1	0.49	2.31	3	2
1:A:151:TRP:NE1	1:A:240:ASP:CG	0.49	2.66	5	1
1:A:143:ALA:O	1:A:152:PHE:CE1	0.49	2.66	15	4
1:A:262:GLY:O	1:A:263:ASP:OD1	0.49	2.31	9	4
1:A:257:ALA:HB3	1:A:271:ILE:CG1	0.49	2.38	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:ARG:CZ	1:A:240:ASP:OD2	0.48	2.60	20	1
1:A:214:TRP:CD2	1:A:214:TRP:C	0.48	2.82	13	1
1:A:271:ILE:HG22	1:A:273:PHE:O	0.48	2.08	20	1
1:A:274:VAL:O	1:A:277:VAL:HG23	0.48	2.09	11	6
1:A:144:ARG:NH1	1:A:151:TRP:NE1	0.48	2.62	15	1
1:A:147:ASN:N	1:A:147:ASN:ND2	0.48	2.61	16	1
1:A:214:TRP:CD1	1:A:253:ARG:NH2	0.48	2.80	18	1
1:A:205:ARG:HH21	1:A:280:ILE:HG21	0.48	1.69	17	1
1:A:157:VAL:CG2	1:A:158:ARG:N	0.48	2.77	14	1
1:A:226:ASN:OD1	1:A:238:TRP:CZ2	0.48	2.66	4	1
1:A:261:LEU:C	1:A:263:ASP:N	0.48	2.66	4	1
1:A:151:TRP:CE2	1:A:240:ASP:OD2	0.48	2.67	5	1
1:A:213:LYS:O	1:A:216:ASP:N	0.48	2.47	9	2
1:A:157:VAL:HG23	1:A:158:ARG:N	0.48	2.23	14	1
1:A:217:LEU:HD22	1:A:277:VAL:HG11	0.47	1.85	15	1
1:A:138:ASN:C	1:A:155:GLN:NE2	0.47	2.68	7	1
1:A:237:PHE:CE2	2:B:653:GLY:C	0.47	2.88	1	1
1:A:136:LYS:N	1:A:139:GLU:OE2	0.47	2.43	8	1
1:A:245:ARG:NH2	1:A:247:ARG:NH1	0.47	2.63	14	1
1:A:213:LYS:NZ	1:A:216:ASP:OD2	0.47	2.47	14	1
1:A:196:VAL:O	1:A:196:VAL:HG13	0.47	2.08	15	3
1:A:209:ARG:CG	1:A:210:THR:N	0.47	2.77	3	2
1:A:235:ARG:C	2:B:652:ALA:O	0.47	2.53	10	18
1:A:214:TRP:CZ3	1:A:246:LYS:NZ	0.47	2.83	2	1
1:A:214:TRP:O	1:A:214:TRP:CE3	0.47	2.67	13	1
1:A:214:TRP:CZ3	1:A:253:ARG:NH2	0.47	2.83	16	1
1:A:274:VAL:O	1:A:277:VAL:CG2	0.46	2.64	12	6
1:A:235:ARG:O	2:B:653:GLY:O	0.46	2.34	10	1
1:A:200:ASN:HD22	1:A:200:ASN:N	0.46	2.08	14	9
1:A:206:ALA:HB3	1:A:281:GLU:HB2	0.46	1.87	18	3
1:A:249:THR:HG1	1:A:252:ALA:N	0.46	2.08	13	10
1:A:200:ASN:ND2	1:A:203:ASP:H	0.46	2.08	14	7
1:A:200:ASN:O	1:A:204:VAL:HG23	0.46	2.10	9	2
1:A:138:ASN:CG	1:A:138:ASN:O	0.46	2.55	19	2
1:A:237:PHE:O	1:A:239:TYR:N	0.46	2.48	13	2
1:A:258:ASN:OD1	1:A:258:ASN:N	0.45	2.37	12	1
1:A:224:MET:SD	1:A:280:ILE:CD1	0.45	2.96	1	1
1:A:253:ARG:HH11	1:A:274:VAL:HG21	0.45	1.72	18	1
1:A:236:GLY:C	2:B:652:ALA:O	0.45	2.55	17	6
1:A:200:ASN:ND2	1:A:200:ASN:C	0.45	2.70	18	6
1:A:187:LYS:HE2	1:A:196:VAL:HG22	0.45	1.89	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:ASP:OD1	1:A:280:ILE:HD11	0.45	2.11	7	1
1:A:235:ARG:HG2	2:B:652:ALA:HB3	0.45	1.88	15	1
1:A:135:TYR:CD1	1:A:135:TYR:N	0.45	2.85	10	2
1:A:214:TRP:CG	1:A:215:GLN:N	0.45	2.83	15	4
1:A:272:ILE:HG23	1:A:273:PHE:CD2	0.45	2.47	20	1
1:A:224:MET:HG3	1:A:280:ILE:HD11	0.45	1.87	13	3
2:B:651:SER:O	2:B:652:ALA:HB2	0.45	2.12	14	3
1:A:227:TYR:HH	1:A:269:CYS:HG	0.45	1.53	5	1
1:A:238:TRP:CZ2	2:B:651:SER:OG	0.45	2.69	18	1
1:A:200:ASN:ND2	1:A:200:ASN:N	0.44	2.64	14	9
1:A:135:TYR:N	1:A:135:TYR:CD1	0.44	2.84	1	1
1:A:228:ASN:OD1	2:B:653:GLY:CA	0.44	2.65	17	1
1:A:200:ASN:N	1:A:200:ASN:HD22	0.44	2.09	10	5
1:A:188:TYR:OH	1:A:197:VAL:CB	0.44	2.65	4	1
1:A:198:GLN:N	1:A:198:GLN:OE1	0.44	2.48	20	1
1:A:136:LYS:O	1:A:139:GLU:CB	0.44	2.65	17	3
1:A:207:ARG:NH2	2:B:649:ARG:NH1	0.44	2.65	5	1
1:A:136:LYS:NZ	1:A:139:GLU:OE1	0.44	2.49	9	1
1:A:135:TYR:CE2	1:A:204:VAL:HG12	0.44	2.48	10	2
1:A:230:ASP:C	1:A:231:ASN:OD1	0.44	2.56	13	3
1:A:144:ARG:CZ	1:A:240:ASP:OD2	0.44	2.66	15	1
1:A:198:GLN:NE2	1:A:198:GLN:N	0.44	2.66	5	1
1:A:242:GLU:O	1:A:258:ASN:OD1	0.44	2.35	12	1
1:A:219:VAL:HG22	1:A:246:LYS:NZ	0.44	2.28	9	1
1:A:238:TRP:CZ2	1:A:278:PHE:CD2	0.44	3.05	1	1
1:A:225:LEU:CD1	1:A:271:ILE:HD12	0.43	2.42	10	1
1:A:138:ASN:O	1:A:138:ASN:CG	0.43	2.54	5	1
1:A:135:TYR:CG	1:A:141:VAL:HG11	0.43	2.49	6	4
1:A:153:GLU:CD	2:B:649:ARG:H	0.43	2.15	5	1
1:A:159:VAL:CG1	1:A:159:VAL:O	0.43	2.67	3	2
1:A:135:TYR:CD2	1:A:141:VAL:HG11	0.43	2.48	3	2
1:A:185:HIS:N	1:A:185:HIS:CD2	0.43	2.86	12	2
1:A:205:ARG:HE	1:A:280:ILE:CG2	0.43	2.25	1	1
1:A:261:LEU:O	1:A:262:GLY:C	0.43	2.56	7	3
1:A:238:TRP:CH2	1:A:278:PHE:CG	0.43	3.07	1	1
1:A:249:THR:HG1	1:A:252:ALA:HB3	0.43	1.72	12	2
2:B:650:LYS:O	2:B:651:SER:OG	0.43	2.36	18	1
1:A:207:ARG:CG	2:B:649:ARG:NH1	0.43	2.82	18	1
1:A:224:MET:CG	1:A:280:ILE:HD11	0.43	2.43	13	2
1:A:237:PHE:O	1:A:238:TRP:C	0.43	2.57	13	1
1:A:247:ARG:CZ	1:A:256:TYR:OH	0.42	2.66	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:ASN:N	1:A:200:ASN:ND2	0.42	2.67	10	2
1:A:209:ARG:NE	1:A:281:GLU:CD	0.42	2.73	15	1
1:A:249:THR:N	1:A:252:ALA:O	0.42	2.46	16	1
1:A:267:ASN:OD1	1:A:267:ASN:C	0.42	2.58	10	3
1:A:212:ILE:O	1:A:277:VAL:CG2	0.42	2.68	8	1
1:A:238:TRP:CZ2	1:A:278:PHE:CE2	0.42	3.06	1	1
1:A:255:LEU:HD13	1:A:256:TYR:N	0.42	2.29	11	1
1:A:225:LEU:O	1:A:239:TYR:N	0.42	2.49	13	1
1:A:159:VAL:HG21	1:A:184:TYR:CE1	0.42	2.49	3	2
1:A:198:GLN:CD	1:A:198:GLN:H	0.42	2.18	14	1
1:A:135:TYR:OH	1:A:204:VAL:O	0.42	2.30	10	2
1:A:235:ARG:HB3	2:B:652:ALA:HB3	0.42	1.90	19	1
1:A:184:TYR:N	1:A:184:TYR:CD1	0.42	2.87	5	1
1:A:237:PHE:CZ	1:A:238:TRP:CE3	0.42	3.08	15	1
1:A:141:VAL:HG12	1:A:206:ALA:HA	0.42	1.91	5	1
1:A:187:LYS:HZ3	1:A:195:GLY:C	0.42	2.15	16	1
1:A:185:HIS:CD2	1:A:185:HIS:N	0.41	2.87	1	1
2:B:650:LYS:C	2:B:651:SER:OG	0.41	2.56	18	1
1:A:151:TRP:NE1	1:A:240:ASP:OD1	0.41	2.54	5	1
1:A:194:ASN:ND2	1:A:197:VAL:HG22	0.41	2.30	5	1
1:A:187:LYS:NZ	1:A:195:GLY:C	0.41	2.74	16	2
1:A:214:TRP:CZ3	1:A:255:LEU:HD11	0.41	2.51	5	1
1:A:218:GLU:C	1:A:246:LYS:HZ1	0.41	2.19	9	1
1:A:200:ASN:HD22	1:A:200:ASN:C	0.41	2.19	18	2
1:A:182:VAL:HG23	1:A:184:TYR:CE2	0.41	2.51	10	1
1:A:223:VAL:O	1:A:241:ALA:O	0.41	2.38	8	2
1:A:226:ASN:ND2	1:A:238:TRP:CE2	0.41	2.86	4	1
1:A:200:ASN:C	1:A:200:ASN:HD22	0.41	2.18	3	1
1:A:213:LYS:O	1:A:214:TRP:C	0.41	2.59	9	1
1:A:200:ASN:ND2	1:A:200:ASN:H	0.41	2.14	14	1
1:A:187:LYS:CE	1:A:195:GLY:O	0.41	2.69	10	1
1:A:272:ILE:CG2	1:A:273:PHE:CE2	0.41	3.04	20	1
1:A:197:VAL:CA	1:A:198:GLN:NE2	0.40	2.84	17	1
1:A:235:ARG:HE	2:B:652:ALA:HB3	0.40	1.76	4	1
1:A:188:TYR:CD1	1:A:188:TYR:N	0.40	2.88	3	1
1:A:208:ALA:HB2	1:A:279:LYS:O	0.40	2.16	18	1
1:A:245:ARG:CB	1:A:245:ARG:NH2	0.40	2.85	15	1
1:A:196:VAL:CG1	1:A:196:VAL:O	0.40	2.70	1	1
1:A:242:GLU:O	1:A:257:ALA:HB1	0.40	2.16	10	1
1:A:200:ASN:HD21	1:A:203:ASP:CG	0.40	2.19	14	1
1:A:200:ASN:C	1:A:200:ASN:ND2	0.40	2.75	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:ALA:CB	1:A:279:LYS:O	0.40	2.70	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	127/152 (84%)	121±1 (95±1%)	5±1 (4±1%)	1±0 (1±0%)	29	74
2	B	6/16 (38%)	5±1 (87±10%)	1±1 (11±11%)	0±0 (2±6%)	11	48
All	All	2660/3360 (79%)	2526 (95%)	111 (4%)	23 (1%)	26	73

All 4 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	238	TRP	19
2	B	651	SER	2
2	B	653	GLY	1
1	A	262	GLY	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	114/136 (84%)	107±2 (94±1%)	7±2 (6±1%)	26	72
2	B	4/10 (40%)	4±0 (98±8%)	0±0 (2±8%)	59	93
All	All	2360/2920 (81%)	2212 (94%)	148 (6%)	27	72

All 26 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	152	PHE	20
1	A	200	ASN	19
1	A	282	ARG	17
1	A	136	LYS	16
1	A	225	LEU	12
1	A	157	VAL	11
1	A	278	PHE	9
1	A	160	THR	7
1	A	214	TRP	7
1	A	198	GLN	4
1	A	279	LYS	4
1	A	209	ARG	4
1	A	138	ASN	3
2	B	651	SER	2
1	A	231	ASN	2
1	A	217	LEU	1
1	A	255	LEU	1
1	A	280	ILE	1
1	A	251	THR	1
1	A	258	ASN	1
1	A	158	ARG	1
1	A	155	GLN	1
1	A	144	ARG	1
1	A	137	VAL	1
1	A	266	LEU	1
1	A	269	CYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates 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 64% for the well-defined parts and 62% for the entire structure.

7.1 Chemical shift list 1

File name: 5iay_cs.str

Chemical shift list name: *data.txt.bak*

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	1464
Number of shifts mapped to atoms	1464
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	137	-0.34 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	125	-0.04 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	6	1.75 ± 1.69	None needed (imprecise)
^{15}N	141	-0.29 ± 0.40	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 64%, i.e. 1108 atoms were assigned a chemical shift out of a possible 1742. 21 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	471/659 (71%)	234/263 (89%)	122/266 (46%)	115/130 (88%)
Sidechain	590/939 (63%)	355/547 (65%)	225/329 (68%)	10/63 (16%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	47/144 (33%)	31/74 (42%)	16/65 (25%)	0/5 (0%)
Overall	1108/1742 (64%)	620/884 (70%)	363/660 (55%)	125/198 (63%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 1326 atoms were assigned a chemical shift out of a possible 2144. 23 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	570/824 (69%)	286/328 (87%)	143/336 (43%)	141/160 (88%)
Sidechain	702/1164 (60%)	432/684 (63%)	260/405 (64%)	10/75 (13%)
Aromatic	54/156 (35%)	37/80 (46%)	16/70 (23%)	1/6 (17%)
Overall	1326/2144 (62%)	755/1092 (69%)	419/811 (52%)	152/241 (63%)

7.1.4 Statistically unusual chemical shifts ⓘ

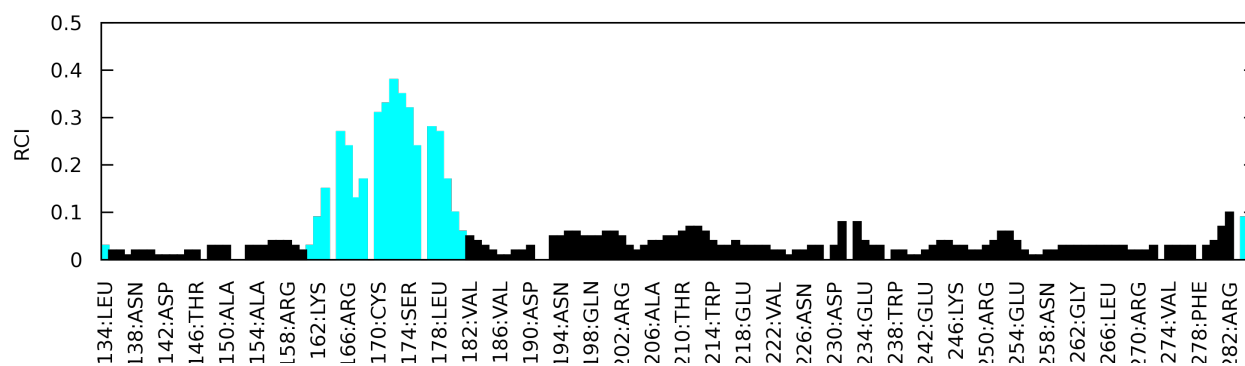
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	181	ASP	C	54.24	185.29 – 167.59	-69.0
1	A	263	ASP	C	54.34	185.29 – 167.59	-69.0
2	B	647	TRP	HE1	3.29	12.85 – 7.35	-12.4
1	A	226	ASN	HB2	0.31	4.36 – 1.26	-8.1
1	A	226	ASN	HB3	0.31	4.41 – 1.11	-7.4
2	B	647	TRP	HE3	10.14	9.33 – 5.33	7.0
1	A	144	ARG	HG2	0.03	2.92 – 0.22	-5.7
1	A	235	ARG	CG	33.94	33.23 – 21.23	5.6
1	A	144	ARG	HG3	0.03	3.00 – 0.10	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

