Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 12:59 AM BST

PDB ID	:	2LAG
Title	:	Structure of the 44 kDa complex of interferon-alpha2 with the extracellular part of IFNAR2 obtained by 2D-double difference NOESY
Authors	:	Nudelman, I.; Akabayov, S.R.; Scherf, T.; Anglister, J.
Deposited on	:	2011-03-13

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

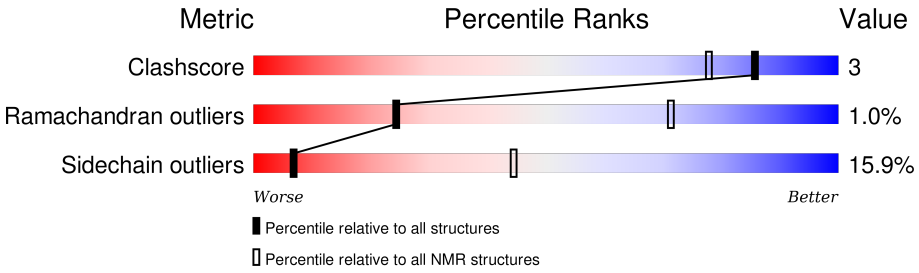
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

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

The overall completeness of chemical shifts assignment is 36%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	212	75% 22%
2	A	165	80% 17%

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	B:5-B:212, A:1-A:160 (368)	0.38	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6052 atoms, of which 2993 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interferon alpha/beta receptor 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	B	212	3356	1094	1647	270	335	10	0

- Molecule 2 is a protein called Interferon alpha-2.

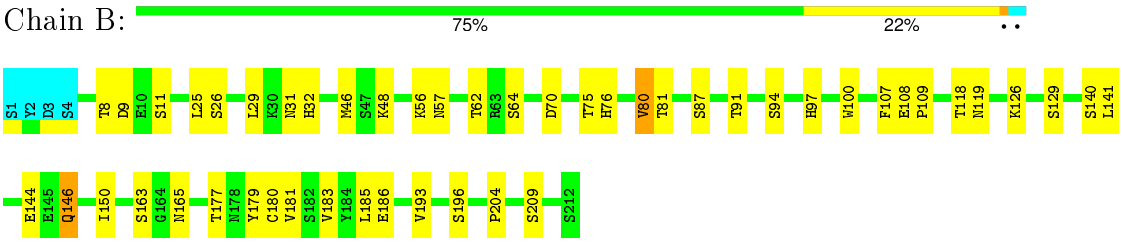
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	165	2696	860	1346	227	254	9	0

4 Residue-property plots (i)

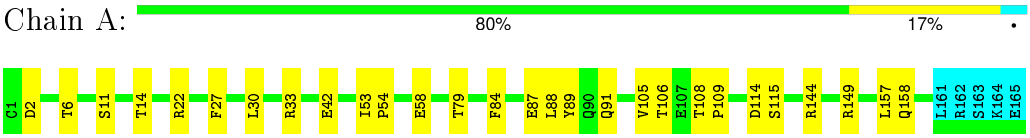
4.1 Average score per residue in the NMR ensemble

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: Interferon alpha/beta receptor 2



• Molecule 2: Interferon alpha-2

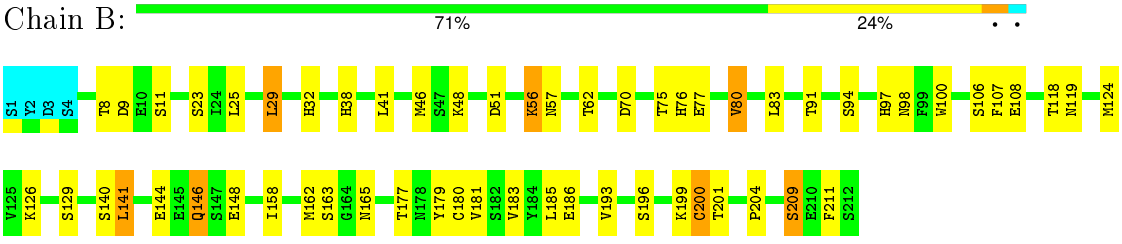


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

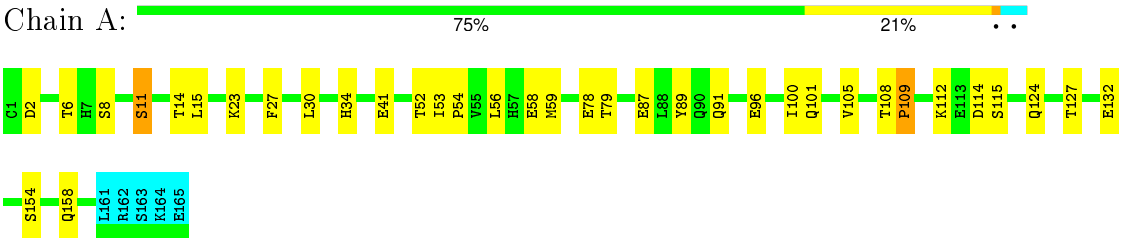
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Interferon alpha/beta receptor 2



• Molecule 2: Interferon alpha-2

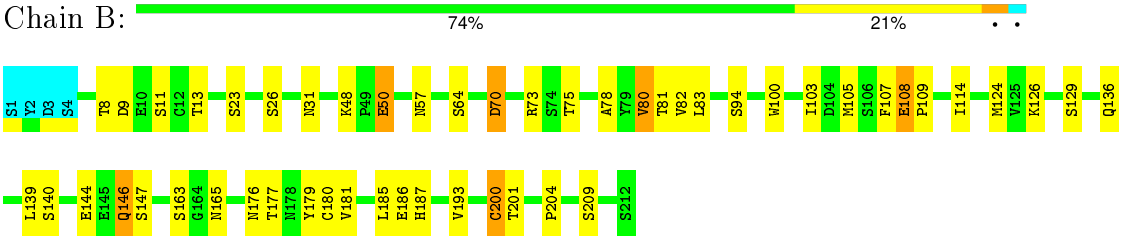
Chain A:



4.2.2 Score per residue for model 2

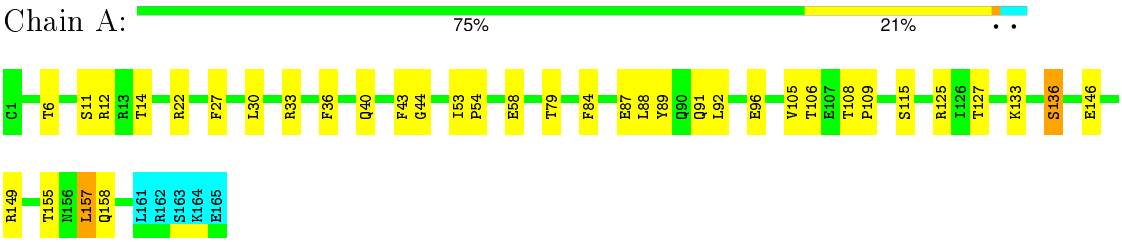
- Molecule 1: Interferon alpha/beta receptor 2

Chain B:



- Molecule 2: Interferon alpha-2

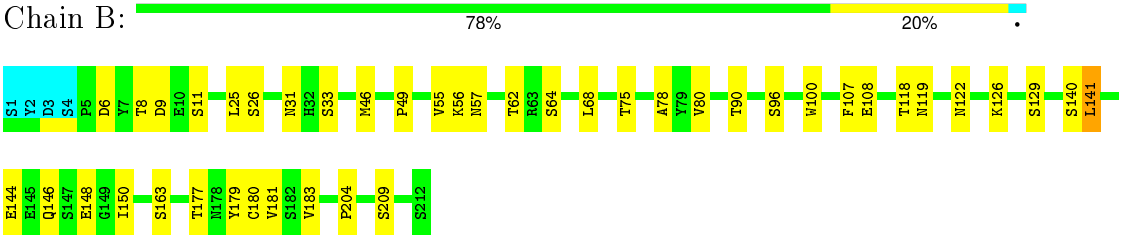
Chain A:



4.2.3 Score per residue for model 3

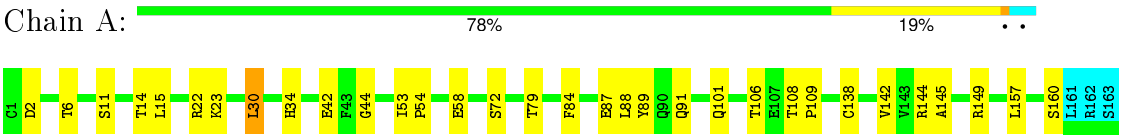
- Molecule 1: Interferon alpha/beta receptor 2

Chain B:



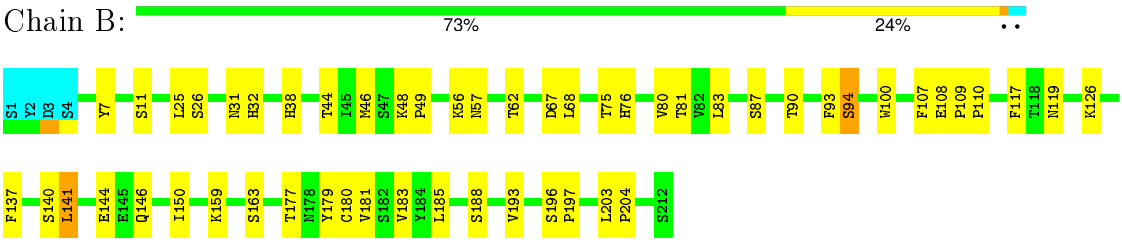
- Molecule 2: Interferon alpha-2

Chain A:

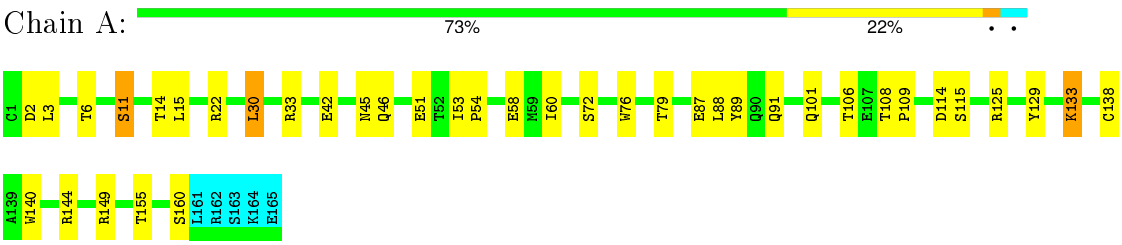


4.2.4 Score per residue for model 4

• Molecule 1: Interferon alpha/beta receptor 2

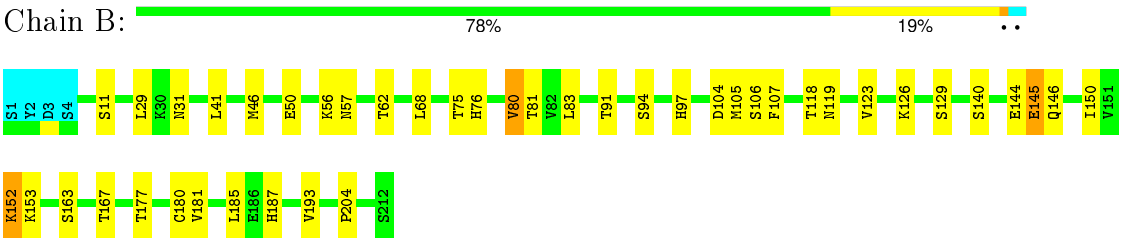


• Molecule 2: Interferon alpha-2

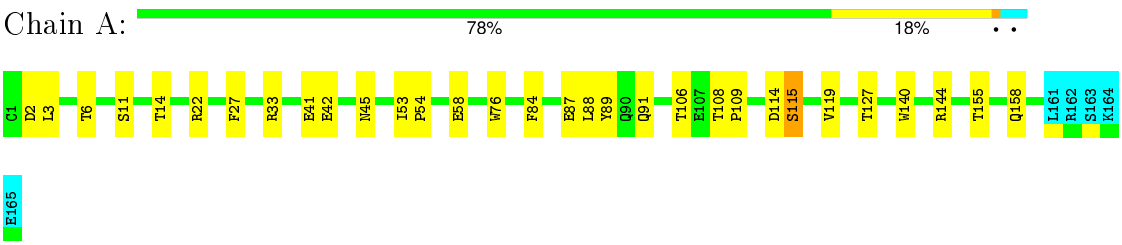


4.2.5 Score per residue for model 5

• Molecule 1: Interferon alpha/beta receptor 2



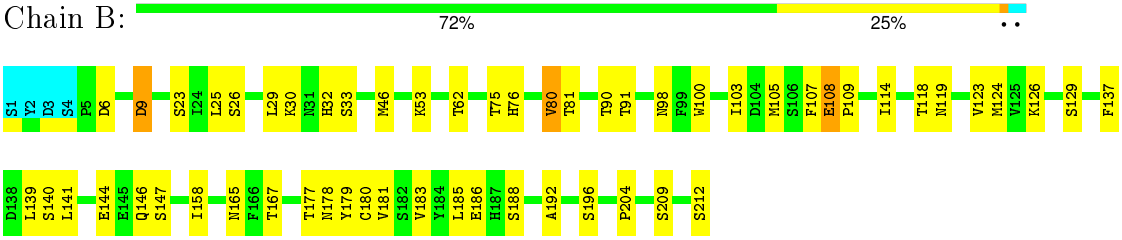
• Molecule 2: Interferon alpha-2



4.2.6 Score per residue for model 6

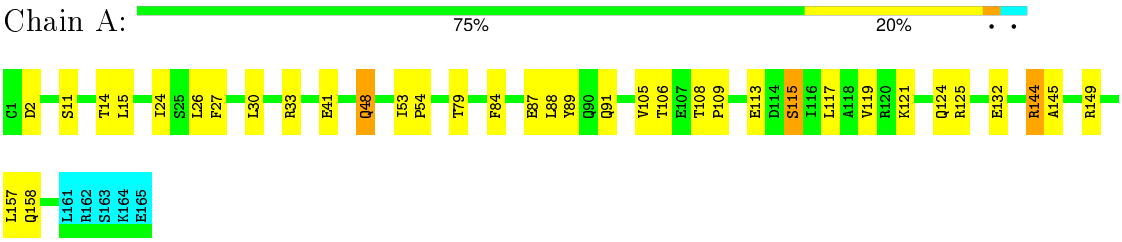
• Molecule 1: Interferon alpha/beta receptor 2

Chain B:



• Molecule 2: Interferon alpha-2

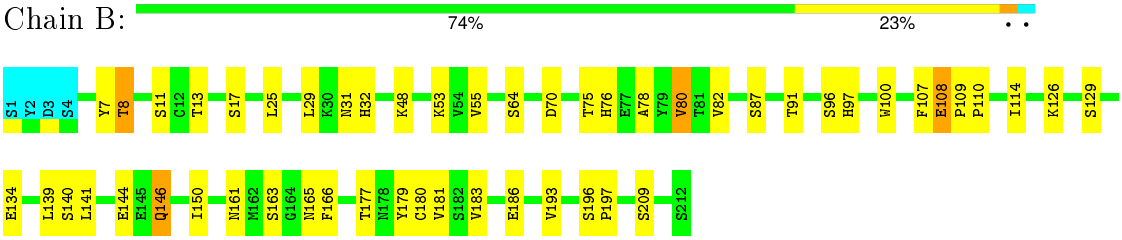
Chain A:



4.2.7 Score per residue for model 7

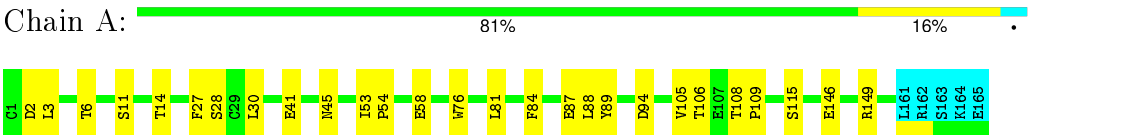
• Molecule 1: Interferon alpha/beta receptor 2

Chain B:



• Molecule 2: Interferon alpha-2

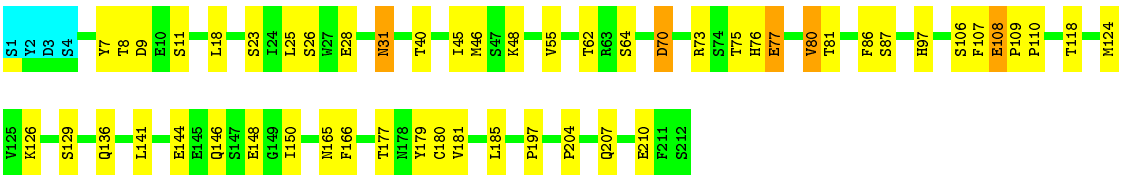
Chain A:



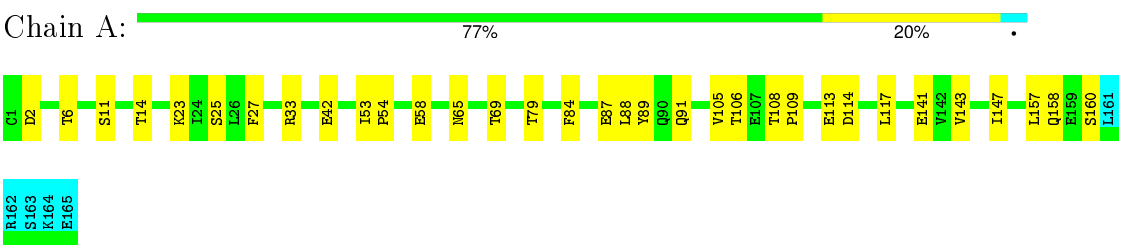
4.2.8 Score per residue for model 8

• Molecule 1: Interferon alpha/beta receptor 2

Chain B:

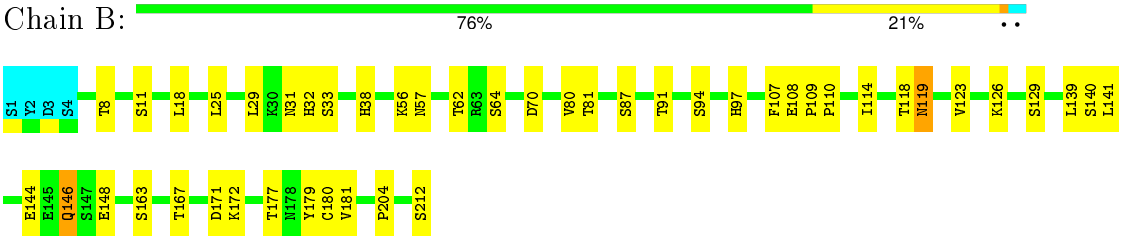


• Molecule 2: Interferon alpha-2

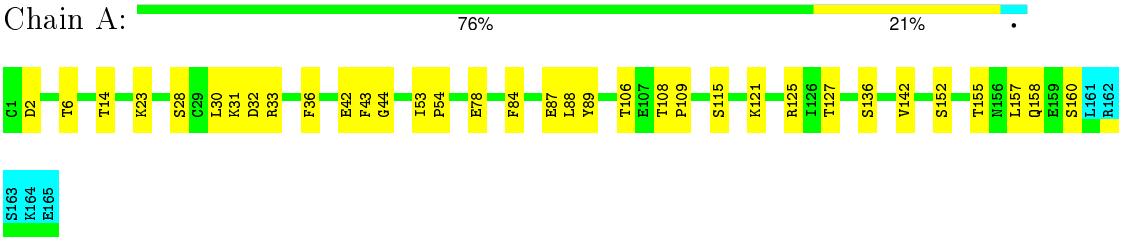


4.2.9 Score per residue for model 9

• Molecule 1: Interferon alpha/beta receptor 2

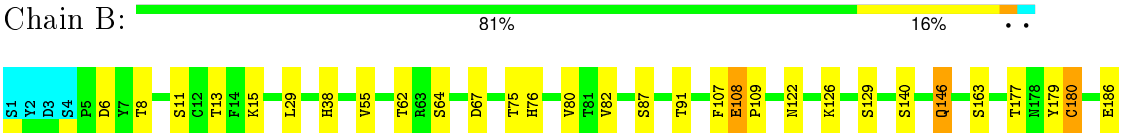


• Molecule 2: Interferon alpha-2

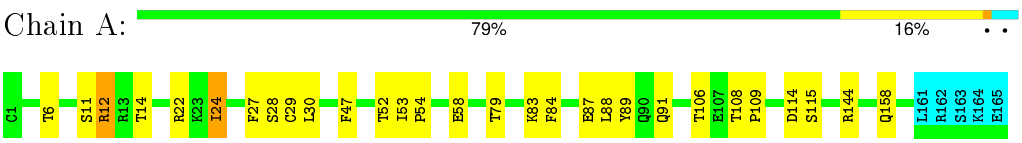


4.2.10 Score per residue for model 10

• Molecule 1: Interferon alpha/beta receptor 2



• Molecule 2: Interferon alpha-2



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
haddock	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)	2lag_cs.str
Number of chemical shift lists	2
Total number of shifts	1950
Number of shifts mapped to atoms	1950
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	36%

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	B	1677	1624	1624	10±3
2	A	1307	1298	1299	8±2
All	All	29840	29220	29230	162

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:MET:SD	1:B:165:ASN:HB2	0.66	2.30	8	4
2:A:22:ARG:HA	2:A:144:ARG:NH2	0.66	2.05	4	2
2:A:11:SER:O	2:A:15:LEU:HG	0.61	1.96	4	2
1:B:146:GLN:O	1:B:179:TYR:HA	0.59	1.97	6	9
1:B:141:LEU:HD11	1:B:183:VAL:HG13	0.59	1.73	3	5
1:B:146:GLN:HA	1:B:150:ILE:O	0.53	2.03	4	5
1:B:179:TYR:CZ	1:B:201:THR:HB	0.53	2.39	2	2
2:A:113:GLU:O	2:A:117:LEU:HG	0.53	2.03	8	2
1:B:144:GLU:O	1:B:181:VAL:HA	0.52	2.05	7	9
2:A:54:PRO:HD3	2:A:105:VAL:CG1	0.51	2.36	8	5
1:B:109:PRO:N	1:B:110:PRO:HD2	0.51	2.20	7	4
1:B:187:HIS:CE1	2:A:12:ARG:HD2	0.50	2.41	10	2
2:A:84:PHE:O	2:A:88:LEU:HG	0.50	2.06	10	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:THR:O	1:B:32:HIS:HB2	0.50	2.06	7	1
1:B:123:VAL:O	1:B:167:THR:HA	0.49	2.08	5	3
1:B:46:MET:HB2	1:B:78:ALA:O	0.49	2.07	3	1
1:B:108:GLU:H	1:B:109:PRO:CD	0.48	2.20	6	4
2:A:133:LYS:HB3	2:A:136:SER:OG	0.48	2.08	2	1
2:A:53:ILE:N	2:A:54:PRO:HD2	0.48	2.24	6	10
2:A:41:GLU:O	2:A:45:ASN:HB2	0.48	2.09	5	2
2:A:22:ARG:HG2	2:A:23:LYS:N	0.48	2.24	3	1
1:B:83:LEU:O	1:B:94:SER:HA	0.47	2.09	2	4
1:B:78:ALA:HB2	1:B:100:TRP:CD1	0.47	2.43	2	2
1:B:114:ILE:HD13	1:B:181:VAL:HB	0.47	1.86	7	1
1:B:56:LYS:O	1:B:57:ASN:HB3	0.47	2.10	3	5
1:B:108:GLU:H	1:B:109:PRO:HD2	0.46	1.71	6	3
2:A:144:ARG:NH1	2:A:145:ALA:HA	0.46	2.25	6	2
2:A:48:GLN:HG3	2:A:157:LEU:HD12	0.46	1.86	6	1
2:A:52:THR:O	2:A:56:LEU:HG	0.46	2.10	1	1
1:B:46:MET:SD	2:A:149:ARG:HB2	0.46	2.51	4	1
1:B:100:TRP:CZ3	2:A:15:LEU:HD13	0.46	2.46	4	3
1:B:180:CYS:HA	1:B:199:LYS:O	0.45	2.11	1	2
1:B:80:VAL:HB	2:A:27:PHE:CE2	0.45	2.47	2	6
2:A:44:GLY:HA2	2:A:157:LEU:HD11	0.45	1.89	9	3
1:B:145:GLU:OE1	1:B:152:LYS:HE2	0.45	2.11	5	1
1:B:171:ASP:O	1:B:172:LYS:HB2	0.44	2.12	9	1
1:B:70:ASP:OD1	1:B:73:ARG:HD3	0.44	2.13	2	2
2:A:109:PRO:O	2:A:112:LYS:HG2	0.44	2.12	1	1
1:B:136:GLN:NE2	2:A:160:SER:HA	0.44	2.27	8	1
2:A:60:ILE:HG23	2:A:88:LEU:HD22	0.44	1.88	4	1
1:B:82:VAL:HB	2:A:27:PHE:CD2	0.44	2.48	7	2
1:B:45:ILE:HB	1:B:77:GLU:OE2	0.44	2.13	8	1
1:B:31:ASN:HD22	1:B:31:ASN:N	0.44	2.11	8	1
1:B:104:ASP:O	1:B:105:MET:HB2	0.43	2.12	5	1
2:A:36:PHE:HA	2:A:125:ARG:NH1	0.43	2.28	2	2
1:B:179:TYR:O	1:B:200:CYS:HA	0.43	2.14	1	2
2:A:96:GLU:O	2:A:100:ILE:HG13	0.43	2.14	1	1
1:B:49:PRO:HB2	2:A:30:LEU:HD12	0.43	1.91	3	2
2:A:65:ASN:O	2:A:69:THR:HG23	0.42	2.13	8	1
2:A:76:TRP:CH2	2:A:140:TRP:HB3	0.42	2.49	5	2
1:B:100:TRP:CH2	2:A:15:LEU:HD22	0.42	2.49	6	1
2:A:41:GLU:HA	2:A:45:ASN:OD1	0.42	2.15	5	1
1:B:188:SER:HB3	2:A:12:ARG:O	0.42	2.14	10	1
2:A:32:ASP:O	2:A:142:VAL:HG21	0.42	2.14	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:129:TYR:CZ	2:A:133:LYS:HE2	0.42	2.49	4	1
2:A:92:LEU:O	2:A:96:GLU:HG2	0.42	2.14	2	1
2:A:45:ASN:O	2:A:46:GLN:HB2	0.42	2.15	4	1
2:A:24:ILE:HD12	2:A:29:CYS:SG	0.42	2.55	10	1
1:B:29:LEU:N	1:B:29:LEU:HD13	0.41	2.30	1	1
1:B:158:ILE:HG22	1:B:162:MET:HB2	0.41	1.92	1	1
2:A:76:TRP:HB2	2:A:81:LEU:HD11	0.41	1.93	7	1
2:A:47:PHE:O	2:A:52:THR:HB	0.41	2.16	10	1
2:A:121:LYS:O	2:A:125:ARG:HG3	0.41	2.16	6	1
2:A:56:LEU:HD22	2:A:154:SER:HB3	0.41	1.93	1	1
1:B:103:ILE:O	1:B:192:ALA:HB2	0.41	2.16	6	1
2:A:115:SER:O	2:A:119:VAL:HG23	0.41	2.15	6	2
1:B:209:SER:HB2	1:B:211:PHE:CZ	0.41	2.51	1	1
2:A:138:CYS:O	2:A:142:VAL:HG23	0.41	2.16	3	1
1:B:9:ASP:HA	1:B:30:LYS:O	0.40	2.16	6	1
1:B:82:VAL:HB	2:A:27:PHE:CE2	0.40	2.51	7	1
1:B:46:MET:SD	2:A:26:LEU:HD21	0.40	2.57	6	1
2:A:143:VAL:O	2:A:147:ILE:HG12	0.40	2.17	8	1
1:B:117:PHE:O	1:B:203:LEU:HB2	0.40	2.16	4	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	B	207/212 (98%)	174±4 (84±2%)	31±4 (15±2%)	3±1 (1±0%)	20	66
2	A	159/165 (96%)	145±2 (91±1%)	13±2 (8±1%)	1±0 (1±0%)	34	78
All	All	3660/3770 (97%)	3190 (87%)	433 (12%)	37 (1%)	24	71

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	109	PRO	10
1	B	108	GLU	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	204	PRO	8
1	B	197	PRO	3
1	B	119	ASN	2
1	B	176	ASN	1
1	B	158	ILE	1
1	B	187	HIS	1
1	B	50	GLU	1
1	B	106	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	B	197/201 (98%)	163±3 (83±2%)	34±3 (17±2%)	6 41
2	A	147/152 (97%)	126±3 (86±2%)	21±3 (14±2%)	8 48
All	All	3440/3530 (97%)	2893 (84%)	547 (16%)	7 44

All 144 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)
2	A	108	THR	10
1	B	80	VAL	10
2	A	87	GLU	10
1	B	107	PHE	10
1	B	126	LYS	10
1	B	177	THR	10
2	A	89	TYR	10
2	A	14	THR	10
2	A	106	THR	9
2	A	11	SER	9
1	B	140	SER	9
1	B	129	SER	9
1	B	180	CYS	9
1	B	75	THR	9
1	B	11	SER	9
2	A	6	THR	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	62	THR	8
2	A	91	GLN	8
2	A	2	ASP	8
2	A	30	LEU	8
2	A	58	GLU	8
2	A	115	SER	8
1	B	163	SER	8
1	B	31	ASN	7
1	B	25	LEU	7
1	B	8	THR	7
2	A	158	GLN	7
2	A	79	THR	7
1	B	76	HIS	7
1	B	185	LEU	6
1	B	193	VAL	6
1	B	29	LEU	6
1	B	81	THR	6
1	B	209	SER	6
1	B	64	SER	6
1	B	118	THR	6
1	B	91	THR	6
2	A	33	ARG	6
1	B	87	SER	5
1	B	186	GLU	5
1	B	141	LEU	5
1	B	70	ASP	5
1	B	9	ASP	5
1	B	119	ASN	5
1	B	97	HIS	5
1	B	196	SER	5
1	B	26	SER	5
1	B	48	LYS	5
2	A	42	GLU	5
1	B	146	GLN	5
2	A	114	ASP	5
2	A	149	ARG	4
1	B	148	GLU	4
1	B	32	HIS	4
2	A	127	THR	4
1	B	139	LEU	4
1	B	38	HIS	4
2	A	155	THR	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	23	SER	4
1	B	55	VAL	4
1	B	114	ILE	3
2	A	3	LEU	3
1	B	13	THR	3
1	B	188	SER	3
1	B	33	SER	3
1	B	90	THR	3
2	A	28	SER	3
2	A	23	LYS	3
1	B	6	ASP	3
2	A	101	GLN	3
1	B	7	TYR	3
1	B	46	MET	3
1	B	68	LEU	3
2	A	160	SER	3
2	A	78	GLU	2
2	A	72	SER	2
1	B	18	LEU	2
1	B	200	CYS	2
2	A	157	LEU	2
2	A	34	HIS	2
2	A	22	ARG	2
2	A	41	GLU	2
2	A	124	GLN	2
1	B	77	GLU	2
2	A	144	ARG	2
1	B	50	GLU	2
2	A	24	ILE	2
2	A	43	PHE	2
1	B	98	ASN	2
1	B	41	LEU	2
1	B	166	PHE	2
1	B	137	PHE	2
1	B	105	MET	2
2	A	146	GLU	2
1	B	94	SER	2
1	B	147	SER	2
1	B	53	LYS	2
1	B	106	SER	2
1	B	122	ASN	2
1	B	96	SER	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	212	SER	2
1	B	67	ASP	2
2	A	136	SER	2
2	A	132	GLU	2
1	B	159	LYS	1
1	B	207	GLN	1
1	B	153	LYS	1
2	A	59	MET	1
1	B	161	ASN	1
2	A	48	GLN	1
1	B	145	GLU	1
1	B	44	THR	1
2	A	125	ARG	1
2	A	25	SER	1
1	B	178	ASN	1
1	B	56	LYS	1
2	A	133	LYS	1
2	A	94	ASP	1
2	A	40	GLN	1
2	A	121	LYS	1
1	B	86	PHE	1
1	B	165	ASN	1
1	B	57	ASN	1
2	A	51	GLU	1
1	B	17	SER	1
2	A	31	LYS	1
1	B	15	LYS	1
1	B	82	VAL	1
2	A	138	CYS	1
2	A	12	ARG	1
1	B	134	GLU	1
2	A	141	GLU	1
2	A	83	LYS	1
1	B	136	GLN	1
1	B	103	ILE	1
2	A	8	SER	1
1	B	210	GLU	1
1	B	203	LEU	1
1	B	51	ASP	1
1	B	152	LYS	1
1	B	93	PHE	1
1	B	40	THR	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	A	152	SER	1
1	B	28	GLU	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 36% for the well-defined parts and 36% for the entire structure.

7.1 Chemical shift list 1

File name: 2lag_cs.str

Chemical shift list name: *assigned.str_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	533
Number of shifts mapped to atoms	533
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	115	-0.05 ± 0.44	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 10%, i.e. 485 atoms were assigned a chemical shift out of a possible 4629. 0 out of 59 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	208/1808 (12%)	96/720 (13%)	0/736 (0%)	112/352 (32%)
Sidechain	250/2387 (10%)	250/1403 (18%)	0/893 (0%)	0/91 (0%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	27/434 (6%)	27/233 (12%)	0/185 (0%)	0/16 (0%)
Overall	485/4629 (10%)	373/2356 (16%)	0/1814 (0%)	112/459 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 499 atoms were assigned a chemical shift out of a possible 4745. 0 out of 60 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	213/1853 (11%)	98/738 (13%)	0/754 (0%)	115/361 (32%)
Sidechain	259/2450 (11%)	259/1441 (18%)	0/914 (0%)	0/95 (0%)
Aromatic	27/442 (6%)	27/237 (11%)	0/189 (0%)	0/16 (0%)
Overall	499/4745 (11%)	384/2416 (16%)	0/1857 (0%)	115/472 (24%)

7.1.4 Statistically unusual chemical shifts (i)

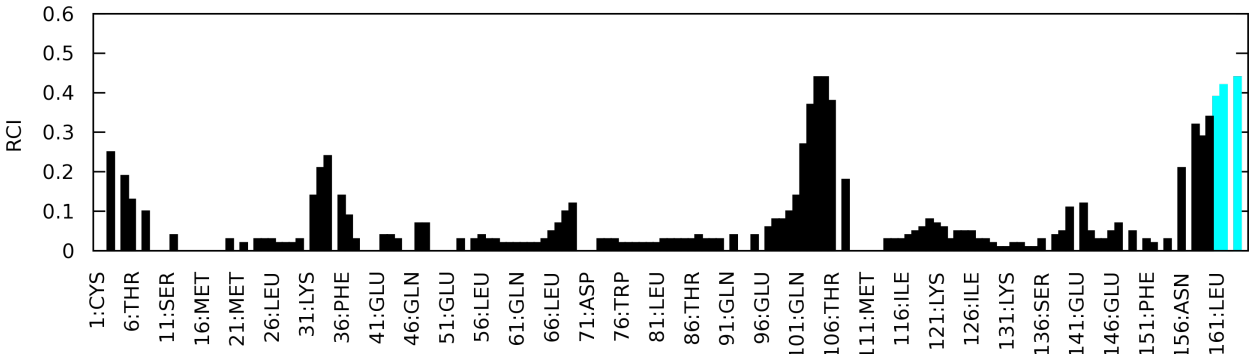
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	140	TRP	H	17.32	12.24 – 4.34	11.4
1	A	116	ILE	H	1.96	11.73 – 4.83	-9.2
1	A	131	LYS	HG2	-0.75	2.67 – 0.07	-8.1
1	A	75	ALA	HB3	-0.41	2.61 – 0.11	-7.1
1	A	75	ALA	HB2	-0.41	2.61 – 0.11	-7.1
1	A	75	ALA	HB1	-0.41	2.61 – 0.11	-7.1
1	A	104	GLY	H	12.35	11.63 – 5.03	6.1
1	A	133	LYS	HD3	0.38	2.75 – 0.45	-5.3

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: 2lag_cs.str

Chemical shift list name: *assigned.str_2*

7.2.1 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	1417
Number of shifts mapped to atoms	1417
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	170	-0.42 ± 0.29	None needed (< 0.5 ppm)

7.2.3 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 25%, i.e. 1176 atoms were assigned a chemical shift out of a possible 4629. 0 out of 59 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	519/1808 (29%)	351/720 (49%)	0/736 (0%)	168/352 (48%)
Sidechain	589/2387 (25%)	589/1403 (42%)	0/893 (0%)	0/91 (0%)
Aromatic	68/434 (16%)	68/233 (29%)	0/185 (0%)	0/16 (0%)
Overall	1176/4629 (25%)	1008/2356 (43%)	0/1814 (0%)	168/459 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 1186 atoms were assigned a chemical shift out of a possible 4745. 0 out of 60 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	525/1853 (28%)	355/738 (48%)	0/754 (0%)	170/361 (47%)
Sidechain	593/2450 (24%)	593/1441 (41%)	0/914 (0%)	0/95 (0%)
Aromatic	68/442 (15%)	68/237 (29%)	0/189 (0%)	0/16 (0%)
Overall	1186/4745 (25%)	1016/2416 (42%)	0/1857 (0%)	170/472 (36%)

7.2.4 Statistically unusual chemical shifts (i)

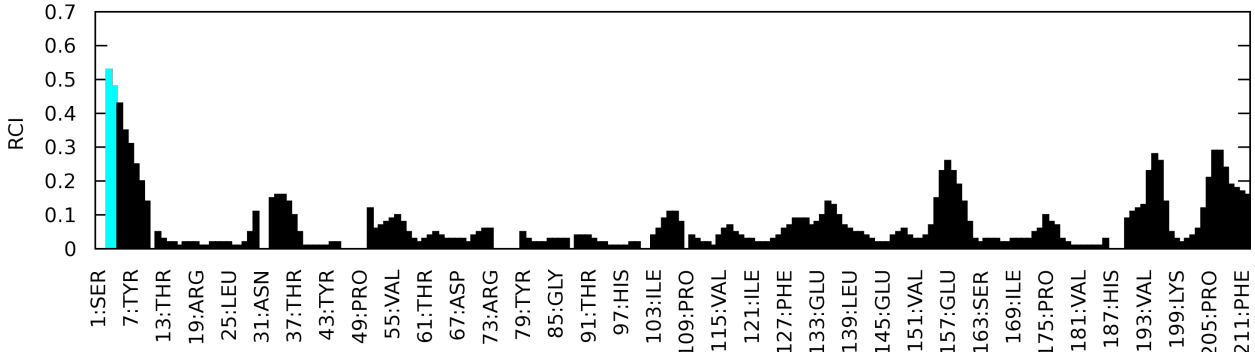
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	68	LEU	HD21	-0.86	2.14 – -0.66	-5.7
2	B	68	LEU	HD23	-0.86	2.14 – -0.66	-5.7
2	B	68	LEU	HD22	-0.86	2.14 – -0.66	-5.7

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 B:


RCI
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1:SER
7:TYR
13:THR
19:ARG
25:LEU
31:ASN
37:THR
43:TYR
49:PRO
55:VAL
61:THR
67:ASP
73:ARG
79:TYR
85:GLY
91:THR
97:HIS
103:ILE
109:PRO
115:VAL
121:ILE
127:PHE
133:GLU
139:LEU
145:GLU
151:VAL
157:GLU
163:SER
169:ILE
175:PRO
181:VAL
187:HIS
193:VAL
199:LYS
205:PRO
211:PHE