wwPDB NMR Structure Validation Summary Report (i)

Apr 20, 2024 – 09:08 AM EDT

PDB ID	:	5JTL
BMRB ID	:	30080
Title	:	The structure of chaperone SecB in complex with unstructured proPhoA
Authors	:	Huang, C.; Saio, T.; Rossi, P.; Kalodimos, C.G.
Deposited on	:	2016-05-09

This is a wwPDB NMR Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

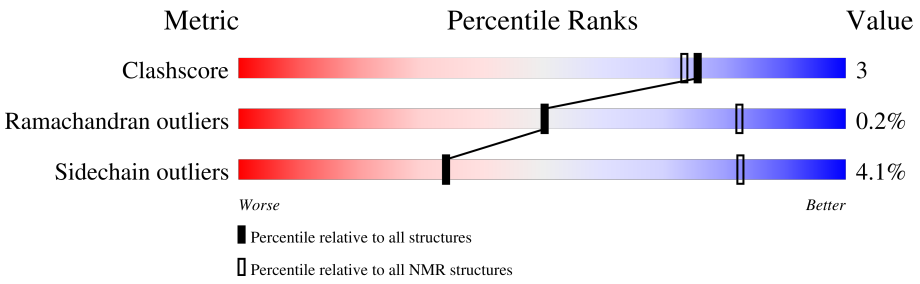
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 13%.

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	155	68% • 30%
1	B	155	73% 6% 21%
1	C	155	69% • 27%
1	D	155	75% 5% 19%
2	E	471	• 99%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:12-A:85, A:98-A:131, B:11-B:132, C:11-C:86, C:97-C:133, D:10-D:134, E:290-E:292 (471)	1.75	13

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 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16399 atoms, of which 8079 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein-export protein SecB.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	155	2367	762	1155	198	243	9	0
1	B	155	2367	762	1155	198	243	9	0
1	C	155	2367	762	1155	198	243	9	0
1	D	155	2367	762	1155	198	243	9	0

- Molecule 2 is a protein called Alkaline phosphatase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	E	471	6931	2154	3459	609	696	13	0

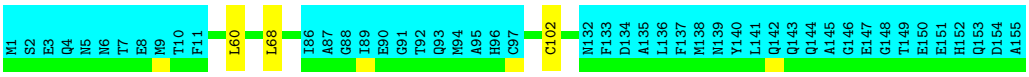
4 Residue-property plots (i)

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.

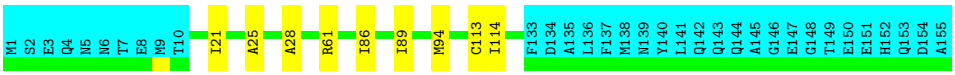
- Molecule 1: Protein-export protein SecB

Chain A:



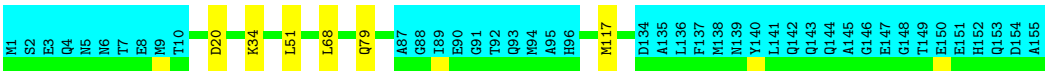
- Molecule 1: Protein-export protein SecB

Chain B:



- Molecule 1: Protein-export protein SecB

Chain C:

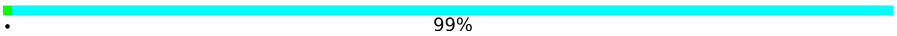


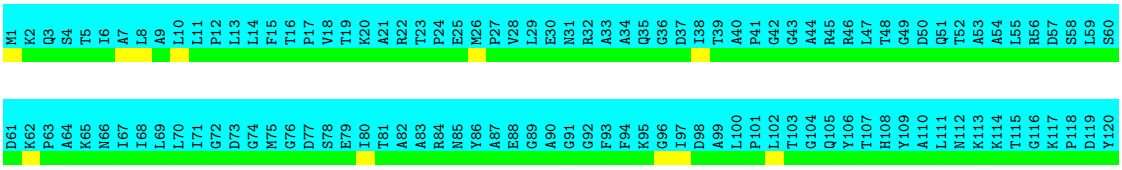
- Molecule 1: Protein-export protein SecB

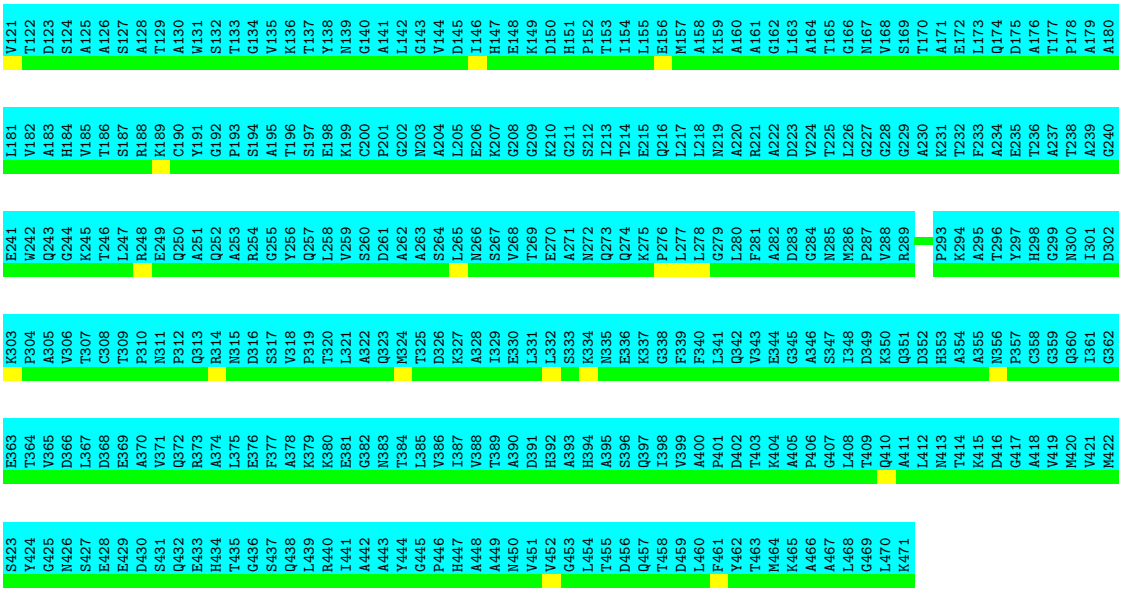
Chain D:

- Molecule 2: Alkaline phosphatase

Chain E:





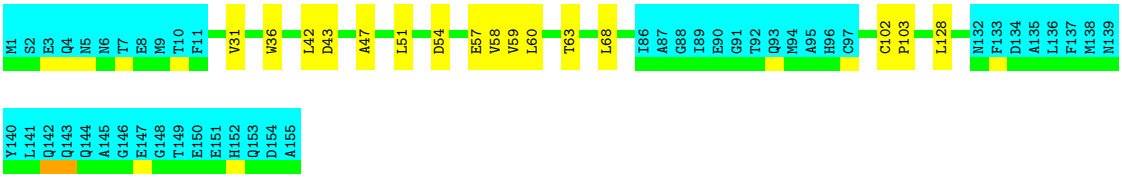


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Protein-export protein SecB

Chain A:

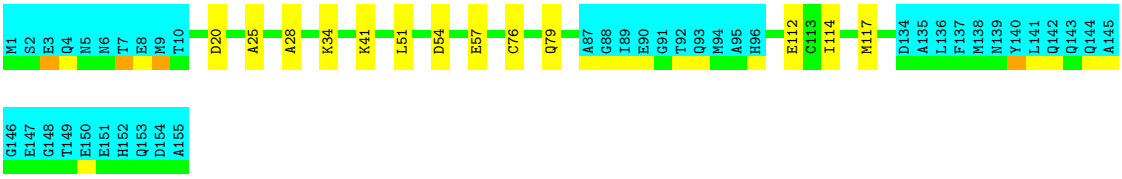


- Molecule 1: Protein-export protein SecB

Chain B:

- Molecule 1: Protein-export protein SecB

Chain C:

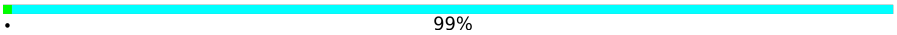


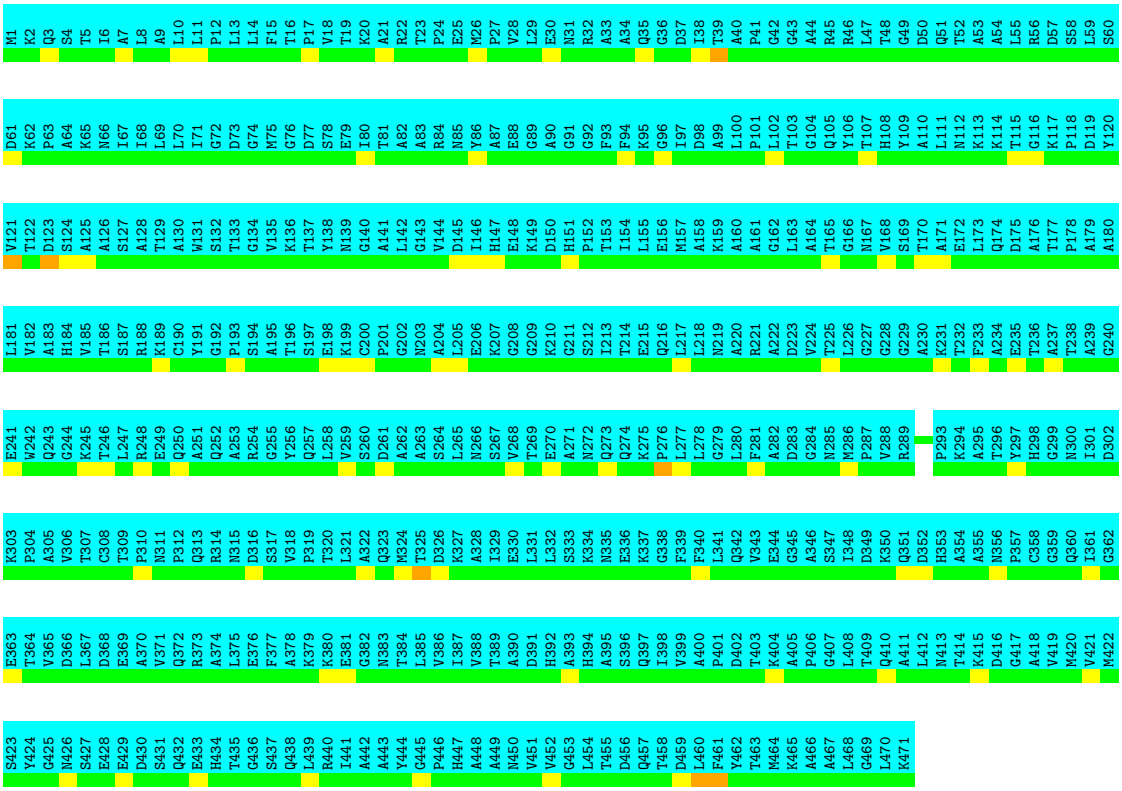
- Molecule 1: Protein-export protein SecB

Chain D:

- Molecule 2: Alkaline phosphatase

Chain E:





5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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	5
Total number of shifts	6416
Number of shifts mapped to atoms	6416
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.87±0.01	0±0/865 (0.0± 0.0%)	0.64±0.01	0±0/1182 (0.0± 0.0%)
1	B	0.88±0.02	0±0/969 (0.0± 0.0%)	0.63±0.02	0±0/1322 (0.0± 0.0%)
1	C	0.88±0.02	0±0/911 (0.0± 0.0%)	0.64±0.02	0±0/1244 (0.0± 0.0%)
1	D	0.87±0.02	0±0/996 (0.0± 0.0%)	0.63±0.02	0±0/1359 (0.0± 0.0%)
2	E	0.91±0.08	0±0/28 (0.0± 0.0%)	0.65±0.14	0±0/40 (0.0± 0.0%)
All	All	0.87	0/75380 (0.0%)	0.64	2/102940 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	111	ARG	NE-CZ-NH2	-5.55	117.52	120.30	15	1
1	B	101	TYR	CA-CB-CG	5.37	123.60	113.40	8	1

There are no chirality outliers.

There are no planarity outliers.

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	845	830	829	5±3
1	B	947	926	924	8±2
1	C	889	870	869	6±3
1	D	973	946	944	6±2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	E	26	24	24	0±0
All	All	73600	71920	71800	457

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.

5 of 250 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:ALA:HB1	1:B:28:ALA:HB2	0.78	1.53	12	6
1:B:89:ILE:HG21	1:B:97:CYS:SG	0.67	2.29	15	1
1:A:20:ASP:HB3	1:A:79:GLN:HB2	0.66	1.66	5	7
1:A:98:LEU:HA	1:A:102:CYS:SG	0.66	2.31	1	3
1:A:16:ILE:HB	1:C:111:ARG:HH12	0.65	1.51	1	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	108/155 (70%)	102±2 (94±1%)	6±2 (5±1%)	0±0 (0±0%)	54	85
1	B	122/155 (79%)	115±3 (94±2%)	7±3 (6±2%)	0±0 (0±0%)	54	85
1	C	113/155 (73%)	105±2 (93±2%)	8±2 (7±2%)	0±1 (0±1%)	44	80
1	D	125/155 (81%)	119±2 (95±2%)	6±2 (4±2%)	0±0 (0±0%)	54	85
2	E	3/471 (1%)	2±1 (72±24%)	1±1 (22±22%)	0±0 (7±13%)	2	18
All	All	9420/21820 (43%)	8856 (94%)	545 (6%)	19 (0%)	50	82

5 of 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	C	130	PRO	4
2	E	292	GLY	3
1	A	29	PRO	2

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Mol	Chain	Res	Type	Models (Total)
1	C	124	PRO	1
1	C	53	ASP	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	94/132 (71%)	90±2 (96±2%)	4±2 (4±2%)	35 83
1	B	104/132 (79%)	101±2 (97±2%)	3±2 (3±2%)	44 89
1	C	99/132 (75%)	94±2 (95±2%)	5±2 (5±2%)	26 75
1	D	107/132 (81%)	103±1 (96±1%)	4±1 (4±1%)	36 84
2	E	2/359 (1%)	2±0 (82±24%)	0±0 (18±24%)	4 39
All	All	8120/17740 (46%)	7791 (96%)	329 (4%)	34 82

5 of 104 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	60	LEU	20
1	C	117	MET	20
1	D	70	GLU	15
1	C	34	LYS	10
1	C	68	LEU	9

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 23% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1049
Number of shifts mapped to atoms	1049
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	139	0.25 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.85 ± 0.17	Should be checked
$^{13}C'$	137	0.29 ± 0.10	None needed (< 0.5 ppm)
^{15}N	133	-1.15 ± 0.27	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 12%, i.e. 777 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	396/2324 (17%)	97/939 (10%)	202/942 (21%)	97/443 (22%)
Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	777/6330 (12%)	306/3470 (9%)	373/2291 (16%)	98/569 (17%)

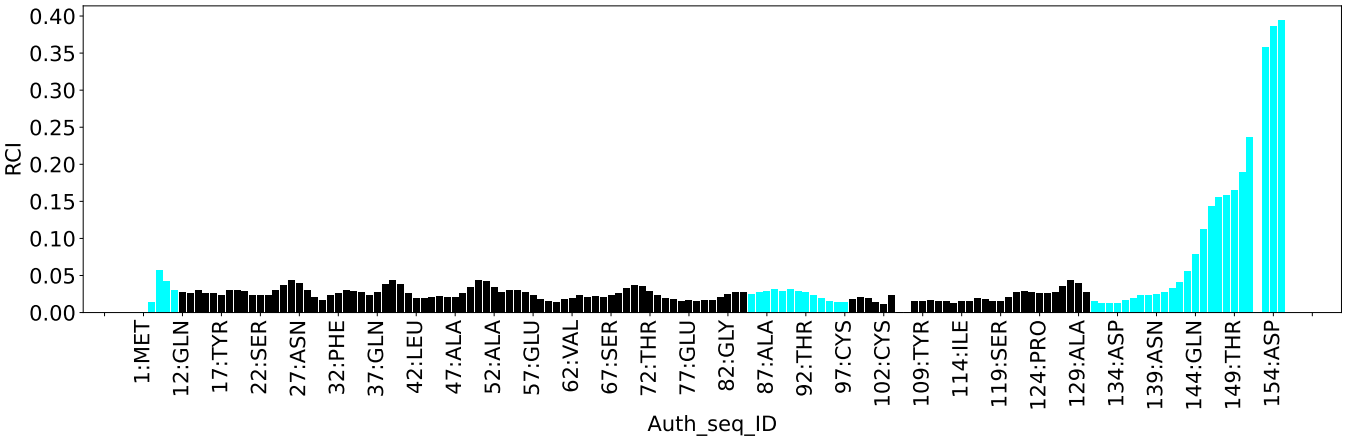
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_2*

7.2.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1044
Number of shifts mapped to atoms	1044
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	140	0.28 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	126	0.79 ± 0.20	Should be checked
$^{13}C'$	135	0.26 ± 0.08	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.25	Should be applied

7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 12%, i.e. 774 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	393/2324 (17%)	96/939 (10%)	201/942 (21%)	96/443 (22%)
Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	774/6330 (12%)	305/3470 (9%)	372/2291 (16%)	97/569 (17%)

7.2.4 Statistically unusual chemical shifts (i)

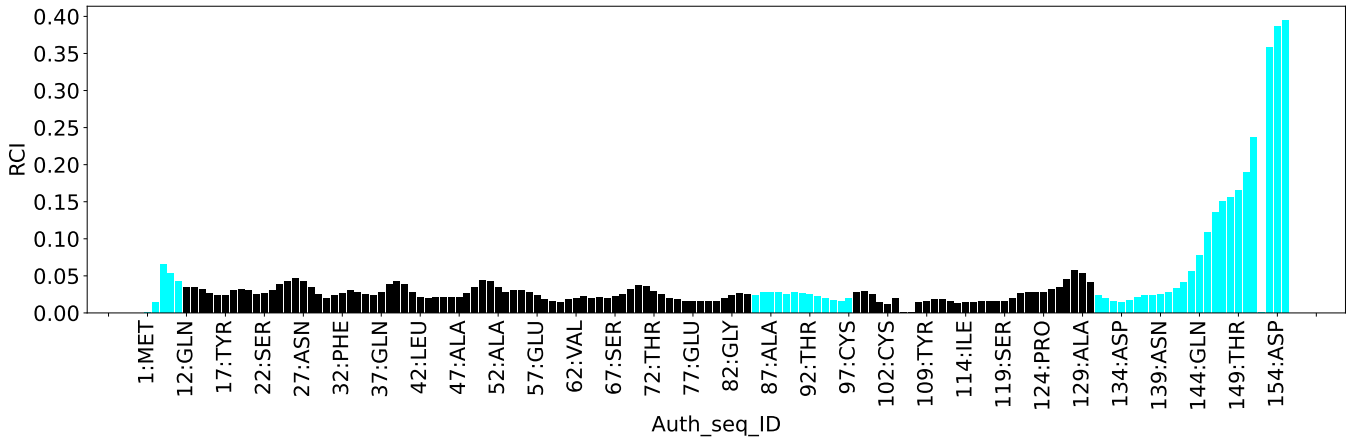
There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_3*

7.3.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1044
Number of shifts mapped to atoms	1044
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

7.3.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	140	0.28 ± 0.08	None needed (< 0.5 ppm)
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$^{13}C'$	135	0.26 ± 0.11	None needed (< 0.5 ppm)
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	Total	^{1}H	^{13}C	^{15}N
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Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	774/6330 (12%)	305/3470 (9%)	372/2291 (16%)	97/569 (17%)

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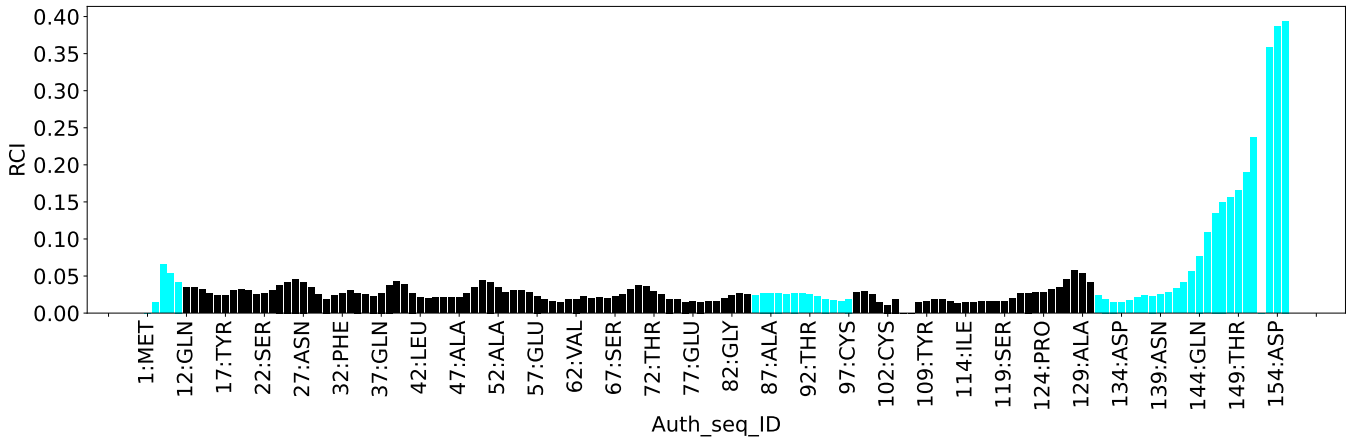
The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted 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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.4 Chemical shift list 4

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_4*

7.4.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1049
Number of shifts mapped to atoms	1049
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

7.4.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	139	0.25 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.84 ± 0.11	Should be checked
$^{13}C'$	137	0.29 ± 0.17	None needed (< 0.5 ppm)
^{15}N	133	-1.15 ± 0.13	Should be applied

7.4.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 12%, i.e. 777 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	396/2324 (17%)	97/939 (10%)	202/942 (21%)	97/443 (22%)
Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	777/6330 (12%)	306/3470 (9%)	373/2291 (16%)	98/569 (17%)

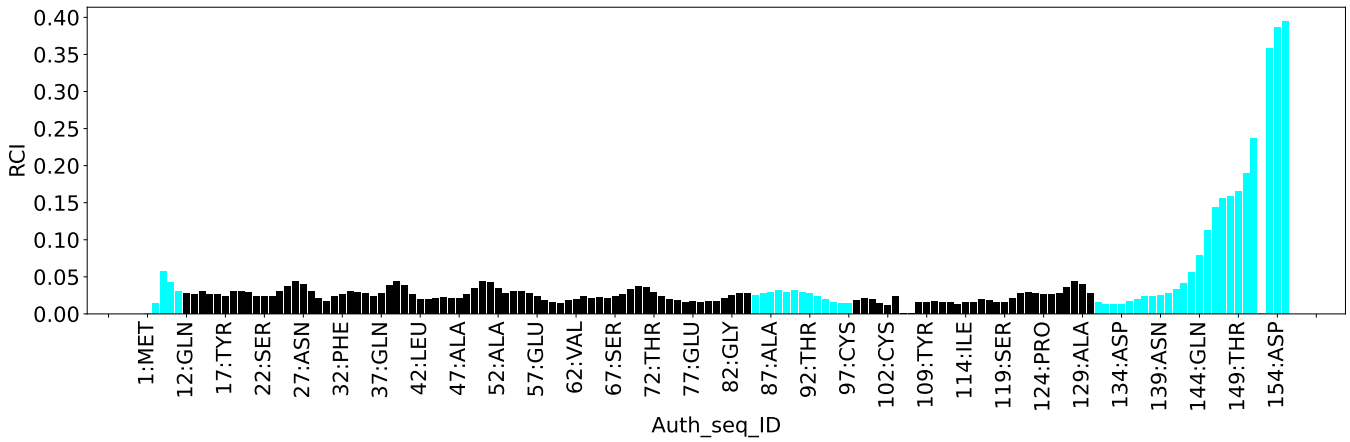
7.4.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.4.5 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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.5 Chemical shift list 5

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_5*

7.5.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2230
Number of shifts mapped to atoms	2230
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

7.5.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	395	-0.41 ± 0.04	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	363	0.38 ± 0.03	None needed (< 0.5 ppm)
$^{13}C'$	90	-0.55 ± 0.05	Should be applied
^{15}N	390	-0.79 ± 0.09	Should be applied

7.5.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 26 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	9/2324 (0%)	3/939 (0%)	3/942 (0%)	3/443 (1%)
Sidechain	10/3464 (0%)	6/2268 (0%)	4/1087 (0%)	0/109 (0%)
Aromatic	7/542 (1%)	6/263 (2%)	0/262 (0%)	1/17 (6%)
Overall	26/6330 (0%)	15/3470 (0%)	7/2291 (0%)	4/569 (1%)

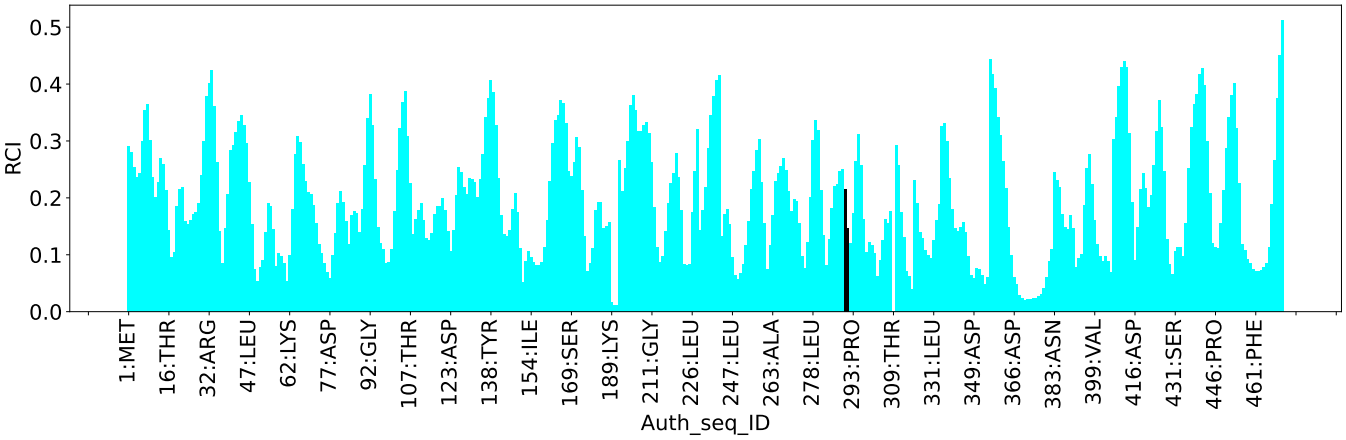
7.5.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.5.5 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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain E:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
1:MET
16:THR
32:ARG
47:LEU
62:LYS
77:ASP
92:GLY
107:THR
123:ASP
138:TYR
154:ILE
169:SER
189:LYS
211:GLY
226:LEU
247:LEU
263:ALA
278:LEU
293:PRO
309:THR
331:LEU
349:ASP
366:ASP
383:ASN
399:VAL
416:ASP
431:SER
446:PRO
461:PHE
Auth_seq_ID