

Full wwPDB NMR Structure Validation Report (i)

Apr 22, 2024 – 01:12 PM JST

:	5ZR0
:	36181
:	Solution structure of peptidyl-prolyl cis/trans isomerase domain of Trigger
	Factor in complex with MBP
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:	2018-04-21
	::

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The 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:

Validation Pipeline (wwPDB-VP) : 2.30.2	MolProbity Percentile statistics wwPDB-RCI PANAV wwPDB-ShiftChecker Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	4.02b-467 20191225.v01 (using entries in the PDB archive December 25th 2019) v_1n_11_5_13_A (Berjanski et al., 2005) Wang et al. (2010) v1.2 Engh & Huber (2001) Parkinson et al. (1996)
· · · · · · · · · · · · · · · · · · ·	Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996) 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 74%.

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 $(\#Entries)$	(# 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	Length Quality of chain								
1	А	142	58%	11%	30%						



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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

	Well-defined (core) p	protein residues	
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:124-A:128, A:150-A:243	0.90	14
	(99)		

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 4 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2079 atoms, of which 1014 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Maltose-binding periplasmic protein, Trigger factor.

Mol	Chain	Residues			Atom	IS			Trace
1	٨	149	Total	С	Η	Ν	0	S	0
1	А	142	2079	664	1014	177	221	3	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	108	GLY	-	expression tag	UNP P0AEX9
А	138	GLY	-	linker	UNP P0AEX9
А	139	SER	-	linker	UNP P0AEX9
А	140	GLY	-	linker	UNP P0AEX9
А	141	SER	-	linker	UNP P0AEX9
А	142	GLY	-	linker	UNP POAEX9
А	143	SER	-	linker	UNP P0AEX9
А	144	GLY	-	linker	UNP P0AEX9
А	145	SER	-	linker	UNP POAEX9
А	146	GLY	-	linker	UNP POAEX9
А	147	SER	-	linker	UNP P0AEX9



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: Maltose-binding periplasmic protein, Trigger factor



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: Maltose-binding periplasmic protein, Trigger factor



4.2.2 Score per residue for model 2

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Chain A: 54% 15% 30%

P218 C108 722 6108 722 6111 722 6111 723 6112 723 6113 723 6114 723 6114 723 6114 723 6117 723 6117 723 6117 723 6117 723 6117 723 6117 723 7120 7249 7123 7249 7123 7249 7123 7249 7133 7249 7133 7249 7133 7249 7133 7249 7133 7149 7133 7149 7133 7149 7149 7149 7149 7149 7149 7149 7149 7149 7149 7149 7149 7144 7149

4.2.3 Score per residue for model 3

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Chain A:	63%	7%	30%
0108 1109 1110 11112 11113 11115 11115 11115 11115 11119 11122 11122	V129 V129 V129 V130 V131 V133 V133 V133 V133 V133 V133	q148 A149 K181 E210 Y221	K227 K227 K238 K238 K238 K238 K238 K238 K238 K238
E247 1249 1249			

4.2.4 Score per residue for model 4

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor



4.2.5 Score per residue for model 5

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor



4.2.6 Score per residue for model 6



Chain A:	57%	13%	30%	-
G108 1109 A1112 A1112 A1113 A1113 A1113 A1114 G1115 T119 T119 T122 T122 T122 T122 T122	412 412 4129 81330 81330 81338 71334 71335 81338 81338 81338 81338 81338 81338 81338 81349 8141 8141 8141 8141 8141 8141 8141 81	S143 C144 C144 S145 S147 Q148 A149 A149 A149 T163	V172 F177 K181 L187 1202	A207 Y221 L226
K227 K228 K228 K228 K229 K228 K243 K243 F244 F244 F244 F244 F245 F245 F245 F245				

4.2.7 Score per residue for model 7

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor



4.2.8 Score per residue for model 8

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Chain A:									5	6%	ó													13	%		30%																				
G108 T100	A 1 1 0	E111	A112	A113	F114	N115 V116	G117	E118	T119	A120	M121	T122	I123	-	W129	S130	N131	I132	D133	113 1 S135	K136	V137	G138	S139	G140 C111	5141 G142	S143	G144 G144	S145	G146	S147	Q148	A149	T150 W151	K154	R163	V164	-	F177	K181	M189		G1 <mark>97</mark>	1202	A207	E210	
V215	100A	1771	K227	-	K232	acon	007NI	K239	V240	E241	E242	R243	E244	L245	P246	E247	L248	T249																													

4.2.9 Score per residue for model 9





4.2.10 Score per residue for model 10

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Chain A:	57%	13%	30%	
6108 1109 11109 11111 11111 11111 11111 11111 11111 1111	W129 W129 N131 1132 1132 1132 1133 1133 N136 N137 N137 N137 S113 S113 S123 S123 S123 S123 S123 S123	0142 8143 8145 8145 8145 8147 8148 8149 8149 8148 8149 8168 1166	V172 F177 F177 I202 A207 A207 E210	Y221 K227
A231 N236 L237 K238 K238 K238 E241 E241 E244 E244 E244 E244 E244 E244				

4.2.11 Score per residue for model 11

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Chain A:	58%	11% •	30%	
6108 1109 1109 6111 6111 6111 6111 6111 6117 6117 611	1129 8130 8131 8132 8133 8133 8133 8133 8133 8133	8147 0148 0149 8159 8159 8159 0162	R103 F177 M189 M194 I202 E210	Y221 K227 G228
K229 N236 N236 N236 N239 K239 K239 K239 K239 F241 F244 F245 F245 F245 F245 F245 F245 F245				

4.2.12 Score per residue for model 12

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

С	h	a	ir	1.	A	•												58	8%)												1	0%		•			3	0%	6						
G108	I109	A110	E111	A112	A113 E114	N115	K116	G117	E118	T119	A120	M121	T122	I123	1120 1120	S130	N131	I132	D133	T134	S135	V137	G138	S139	G140	S141	G142	S143	6144 01710	G146	S147	Q 148	A149	E153	K154	E159	D162 R163	V164		V172	K181	A188	Y221	7770	K227	A231
	K238	K239	V240	E241		E244 1.245	P246	E247	L248	T249																																				

4.2.13 Score per residue for model 13



4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Chain A:	58%	12%	30%	•
C1 08 E1 11 0 E1 11 0 E1 11 1 E1 11 1 E1 11 1 E1 11 1 E1 15 E1 15 E1 15 E1 15 E1 12 E1 12	V1 29 V1 29 V1 29 V1 20 V1 33 V1 33 V1 37 V1 36 V1 36 V1 36 V1 29 V1 20 V1 20 V1 V1 20 V1 20 V1 20 V1 20 V1 20 V1 20 V1 20 V1 20 V1 20 V1 20 V10	142 1442 1443 1145 1145 1149 1149 1149 1165	F177 E178 K181 M189 M189 T202 F211	Y221 K227 L237
K238 V240 V240 E241 E244 E244 E244 E244 E244 E244 E247 E244 T249				

4.2.15 Score per residue for model 15

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Chain A:	57%	13%	30%
6108 1109 1110 6111 61112 7113 7113 6115 6115 7113 7121 7122 7122	P126 W129 W129 W129 W121 F134 F134 F134 F134 F134 F136 V137 C136 G140 G140	G142 5143 6144 5145 6144 6146 8146 8146 8146 8146 8146 8148 8148	N172 F177 K181 M189 E199 E199 E210
K227 K227 A231 A231 L236 L236 K239 K239 K239 K243 F245 F244 F246 F244	L249 T249		

4.2.16 Score per residue for model 16

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Cł	ıa	in	1 1	4	•											60)%														8%	6	•				3	30%)							
G108 I109	A110	E111	A112	A113 5444	N115	K116	G117	E118	T119	A120	M121	T122	I123	P126	W129	S130	T132	D133	T134	S135	K136	V137 2122	6138	S 139 G 140	G140	5141 G142	S143	G144	S145	G146	S147	Q148	A149	V179	F177	M189		R193	F211	Y221	L226	K227	G228	A 230	A231	
L237 K238	-	E242	R243	E244	P246	E247	L248	T249																																						

4.2.17 Score per residue for model 17



4.2.18 Score per residue for model 18

• Molecule 1: Maltose-binding periplasmic protein, Trigger factor



- 4.2.19 Score per residue for model 19
- Molecule 1: Maltose-binding periplasmic protein, Trigger factor

Cha	ain	ı A	\ :											5	579	6												12º	%		•			30	%				
G108 I109	E111	A112 A113	F114	N115 V116	G117	E118	T119	A120	M121 T122	1122 T123		W129	S130	N131	I132	T134	S135	K136	V13/ C138	S139	G140	S141 C142	G142 S143	G144	S145	G146	S147	4148 A149	T150	W151	K154	 R163	V172	E178	K181	F 198	K206 A207	Y221	K227
A231	L237	K238 K739	V240	E241	E243 R243	E244	L245	P246	E247 1 248	T249	0171																												

4.2.20 Score per residue for model 20





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
CYANA	structure calculation	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1275
Number of shifts mapped to atoms	1275
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%



6 Model quality (i)

6.1 Standard geometry (i)

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 (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	А	767	730	728	6 ± 2
All	All	15340	14600	14560	117

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 4.

Atom 1	Atom 2	$Clach(\lambda)$	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:167:ASP:HB2	1:A:238:LYS:HD3	0.66	1.66	18	3
1:A:189:MET:SD	1:A:202:ILE:HD11	0.65	2.31	14	5
1:A:165:THR:HG21	1:A:243:ARG:HB2	0.63	1.70	14	1
1:A:153:GLU:HA	1:A:241:GLU:HA	0.60	1.73	13	7
1:A:154:LYS:HB2	1:A:240:VAL:HB	0.60	1.74	11	7
1:A:172:VAL:HG11	1:A:226:LEU:HD11	0.60	1.72	1	2
1:A:207:ALA:HA	1:A:237:LEU:HB3	0.56	1.76	6	8
1:A:172:VAL:HA	1:A:231:ALA:HA	0.55	1.79	10	15
1:A:154:LYS:HB3	1:A:240:VAL:HB	0.55	1.79	8	2
1:A:164:VAL:HG23	1:A:240:VAL:HA	0.55	1.77	7	4
1:A:159:GLU:H	1:A:162:ASP:HB3	0.54	1.62	9	3
1:A:189:MET:HB3	1:A:202:ILE:HD11	0.53	1.81	1	2
1:A:189:MET:SD	1:A:203:LYS:HG2	0.52	2.44	18	1
1:A:166:ILE:HG21	1:A:202:ILE:HG21	0.52	1.81	10	4

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

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A + a 1	A + 2	$C = c \left(\overset{\circ}{\lambda} \right)$	\mathbf{D} : \mathbf{D} : \mathbf{D}	Mo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:239:LYS:HG3	1:A:241:GLU:H	0.51	1.65	10	2
1:A:159:GLU:HB2	1:A:162:ASP:HB2	0.51	1.82	20	3
1:A:125:GLY:HA3	1:A:194:MET:HA	0.51	1.81	18	1
1:A:165:THR:HG21	1:A:243:ARG:HG3	0.50	1.82	18	1
1:A:151:TRP:HB2	1:A:242:GLU:HA	0.50	1.83	1	2
1:A:227:LYS:HD3	1:A:227:LYS:H	0.50	1.67	16	2
1:A:172:VAL:HG22	1:A:229:LYS:HG3	0.49	1.82	6	1
1:A:164:VAL:HG12	1:A:202:ILE:HD12	0.49	1.84	5	1
1:A:211:PHE:HE2	1:A:237:LEU:HB2	0.47	1.70	1	5
1:A:187:LEU:HD23	1:A:202:ILE:HD13	0.47	1.86	6	1
1:A:168:PHE:HA	1:A:235:ILE:HG21	0.47	1.87	4	1
1:A:151:TRP:HB2	1:A:242:GLU:HB3	0.47	1.85	8	1
1:A:227:LYS:H	1:A:227:LYS:HD2	0.47	1.70	13	2
1:A:189:MET:HE2	1:A:203:LYS:HD3	0.46	1.86	9	1
1:A:210:GLU:HA	1:A:236:ASN:HA	0.46	1.86	20	10
1:A:207:ALA:HB2	1:A:240:VAL:HG13	0.44	1.89	8	2
1:A:194:MET:SD	1:A:194:MET:N	0.44	2.90	5	1
1:A:126:PRO:HG3	1:A:218:PRO:HD2	0.44	1.90	9	1
1:A:166:ILE:HG22	1:A:237:LEU:HD11	0.43	1.90	13	1
1:A:167:ASP:HB3	1:A:235:ILE:HG12	0.43	1.90	7	1
1:A:158:VAL:HB	1:A:203:LYS:HA	0.43	1.90	20	1
1:A:128:ALA:HB2	1:A:222:HIS:NE2	0.42	2.30	4	1
1:A:197:GLY:HA3	1:A:215:VAL:HB	0.42	1.90	8	1
1:A:165:THR:HG21	1:A:243:ARG:HB3	0.42	1.90	13	1
1:A:221:TYR:HB3	1:A:226:LEU:HB3	0.42	1.92	19	1
1:A:163:ARG:HB3	1:A:188:ALA:HA	0.41	1.90	12	1
1:A:193:ARG:HB2	1:A:194:MET:SD	0.41	2.56	4	1
1:A:126:PRO:HB3	1:A:218:PRO:HD2	0.41	1.92	2	1
1:A:126:PRO:HB2	1:A:221:TYR:HB2	0.41	1.92	16	1
1:A:189:MET:SD	1:A:199:GLU:HA	0.40	2.56	15	1
1:A:178:GLU:HA	1:A:181:LYS:HE3	0.40	1.92	19	1
1:A:165:THR:HG21	1:A:243:ARG:HG2	0.40	1.94	2	1
1:A:226:LEU:HD13	1:A:229:LYS:HD3	0.40	1.92	16	1

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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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	99/142~(70%)	89 ± 2 (90 $\pm2\%$)	$9\pm2~(9\pm2\%)$	1±1 (1±1%)	18	66
All	All	1980/2840~(70%)	1783 (90%)	176 (9%)	21 (1%)	18	66

was analysed and the total number of residues.

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	238	LYS	7
1	А	228	GLY	4
1	А	241	GLU	2
1	А	125	GLY	1
1	А	180	GLY	1
1	А	219	GLU	1
1	А	242	GLU	1
1	А	227	LYS	1
1	А	126	PRO	1
1	A	156	GLY	1
1	А	224	GLU	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	А	76/107~(71%)	$69 \pm 1 (91 \pm 2\%)$	$7\pm1 (9\pm2\%)$	13 59
All	All	1520/2140~(71%)	1382 (91%)	138 (9%)	13 59

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	А	227	LYS	20
1	А	221	TYR	15
1	А	181	LYS	15
1	А	163	ARG	14
1	А	177	PHE	14
1	А	242	GLU	11

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Mol	Chain	Res	Type	Models (Total)
1	А	243	ARG	8
1	А	239	LYS	6
1	А	124	ASN	4
1	А	232	LYS	4
1	А	152	LYS	3
1	А	222	HIS	3
1	А	198	PHE	3
1	А	161	GLU	3
1	А	189	MET	2
1	А	238	LYS	2
1	А	154	LYS	2
1	А	240	VAL	1
1	А	226	LEU	1
1	А	194	MET	1
1	А	229	LYS	1
1	А	220	GLU	1
1	А	178	GLU	1
1	А	193	ARG	1
1	А	153	GLU	1
1	А	206	LYS	1

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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 74% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: chemical_shift_set1

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	1275
Number of shifts mapped to atoms	1275
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	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	126	-0.06 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	116	-0.11 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	0		None (insufficient data)
¹⁵ N	119	-0.11 ± 0.41	None needed (< 0.5 ppm)

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 74%, i.e. 951 atoms were assigned a chemical shift out of a possible 1285. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	378/502~(75%)	192/208~(92%)	93/198~(47%)	93/96~(97%)
Sidechain	517/664~(78%)	344/425~(81%)	173/216~(80%)	0/23~(0%)

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	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N	
Aromatic	56/119~(47%)	34/59~(58%)	22/54~(41%)	0/6~(0%)	
Overall	951/1285 (74%)	570/692 (82%)	288/468~(62%)	93/125 (74%)	

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1275 atoms were assigned a chemical shift out of a possible 1774. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	496/722~(69%)	251/300~(84%)	126/284~(44%)	119/138~(86%)
Sidechain	712/911 (78%)	474/587~(81%)	238/296~(80%)	0/28~(0%)
Aromatic	67/141~(48%)	40/70~(57%)	27/64~(42%)	0/7~(0%)
Overall	1275/1774 (72%)	765/957~(80%)	391/644~(61%)	119/173~(69%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (1)

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:



