



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6PSI / pdb\_00006psi  
BMRB ID : 30638  
Title : Structural Basis for Client Recognition and Activity of Hsp40 Chaperones  
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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
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) : 2.49

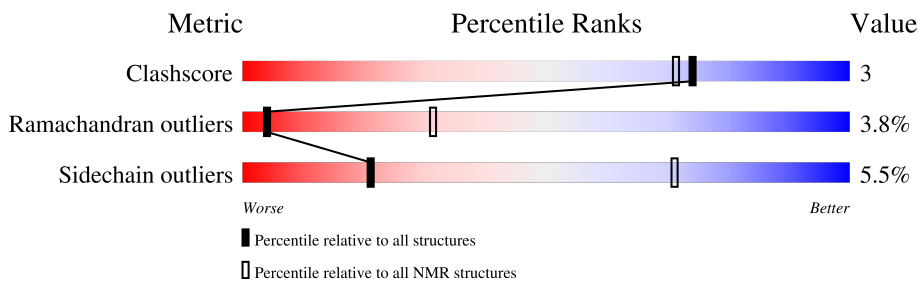
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 23%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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  $\geq 3$ , 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	280	
1	C	280	
2	B	471	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:4-A:108, A:115-A:280, B:1-B:11, B:179-B:185, B:238-B:245, C:3-C:105, C:116-C:280 (565)	2.80	4

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. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15729 atoms, of which 7873 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chaperone protein DnaJ 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	280	4399	1398	2207	393	398	3	0
1	C	280	4399	1398	2207	393	398	3	0

- Molecule 2 is a protein called Alkaline phosphatase.

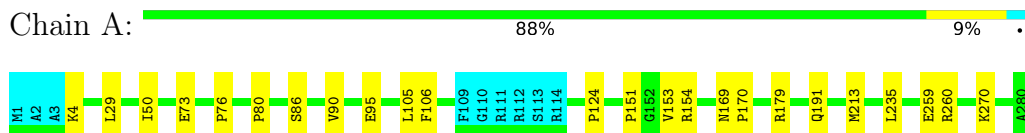
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	471	6931	2154	3459	609	696	13	0

## 4 Residue-property plots i

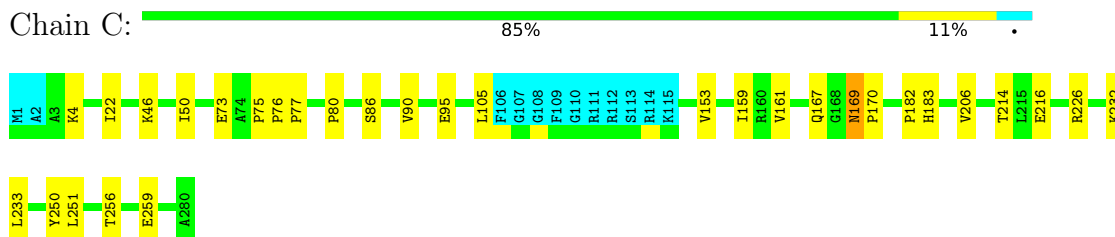
### 4.1 Average score per residue in the NMR ensemble

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.

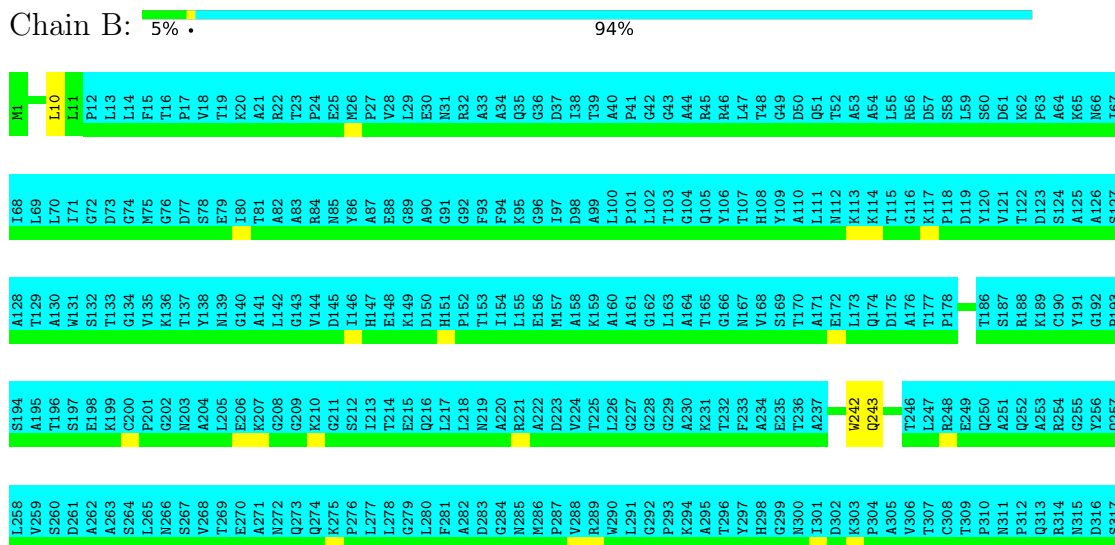
- Molecule 1: Chaperone protein DnaJ 2

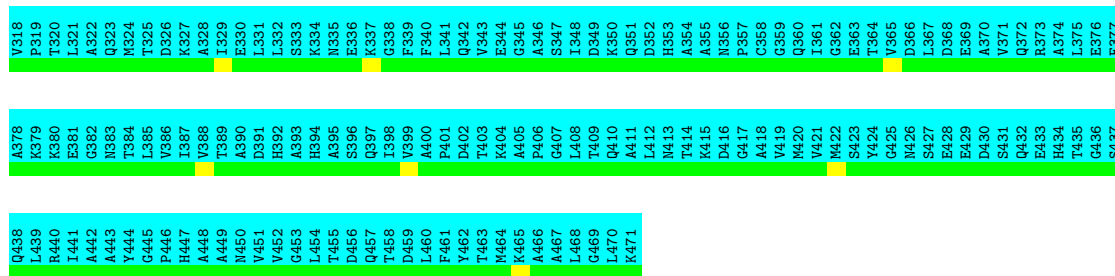


- Molecule 1: Chaperone protein DnaJ 2



- Molecule 2: Alkaline phosphatase

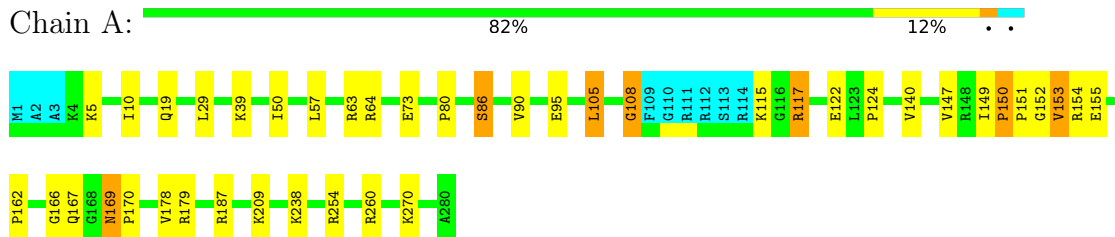




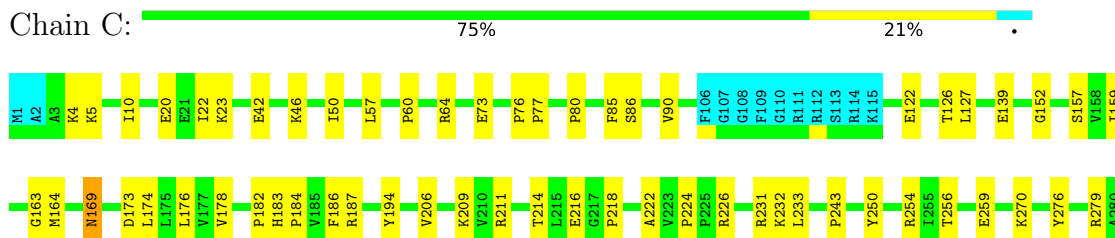
## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

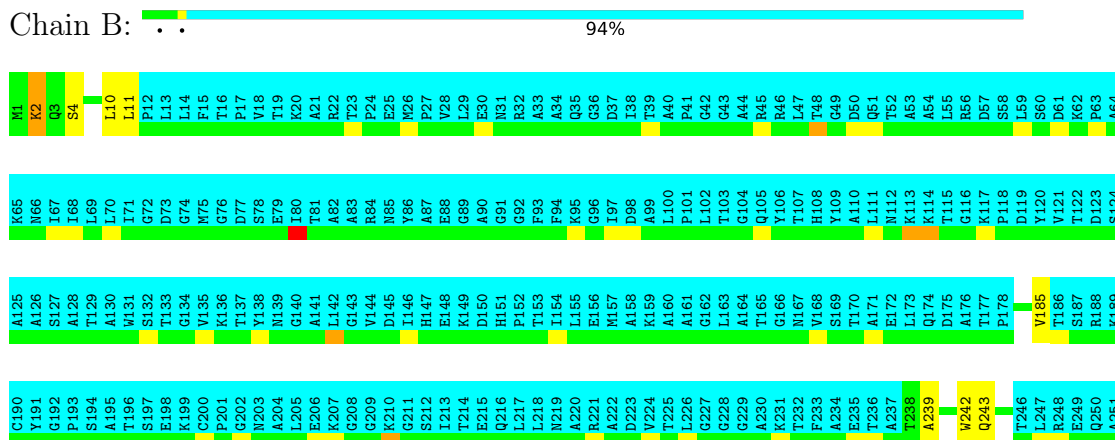
- Molecule 1: Chaperone protein DnaJ 2



- Molecule 1: Chaperone protein DnaJ 2



- Molecule 2: Alkaline phosphatase



Q322	Q252
A253	A254
G255	Y256
S317	L258
V318	V259
F319	S260
T320	D321
L321	A262
A322	A263
Q323	S264
M324	L265
T325	M266
D326	S267
K327	V268
A328	T269
I329	E270
E330	A271
L331	M272
L332	Q273
S333	Q274
K334	K275
A335	P276
S336	L277
K337	L278
G338	G279
F339	L280
F340	F281
L341	F282
Q342	D283
V343	G284
E344	M285
G345	M286
A346	P287
S347	V288
I348	R289
D349	M290
K350	L291
Q351	G292
D352	P293
H353	K294
A354	A295
A355	T296
M356	Y297
P357	H298
C358	G299
G359	N300
Q360	I301
I361	D302
G362	K303
E363	P304
T364	A305
V365	V306
G425	T307
N426	D368
S427	E369
E428	A370
E429	P310
D430	M311
S431	
Q372	P312
R373	Q313
A374	R314
L375	N315
E376	D316
F377	S317
A378	V318
K379	F319
K380	T320
E381	L321
G382	A322
N383	Q323
T384	M324
L385	T325
V386	D326
I387	K327
V388	A328
T389	I329
A390	E330
D391	L331
H392	L332
A393	S333
H394	K334
A395	A335
S396	S336
Q397	K337
I398	G338
V399	F339
A400	F340
P401	L341
D402	Q342
T403	V343
K404	E344
A405	G345
P406	A346
G407	S347
L408	I348
T409	D349
Q410	K350
A411	Q351
L412	D352
N413	H353
T414	A354
K415	A355
D416	M356
G417	P357
A418	C358
V419	G359
M420	Q360
V421	I361
M422	G362
S423	E363
Y424	T364
G425	V365
N426	G425
S427	N426
E428	S427
E429	E428
D430	E429
S431	D430

## 5 Refinement protocol and experimental data overview

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	
TALOS	geometry optimization	

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	2
Total number of shifts	2726
Number of shifts mapped to atoms	2726
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	23%

## 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	1.31±0.03	4±2/2175 ( 0.2± 0.1%)	1.03±0.02	1±2/2949 ( 0.0± 0.1%)
1	C	1.31±0.02	4±2/2151 ( 0.2± 0.1%)	1.03±0.03	1±2/2919 ( 0.0± 0.1%)
2	B	1.37±0.08	0±1/192 ( 0.2± 0.3%)	1.03±0.07	0±0/262 ( 0.0± 0.0%)
All	All	1.31	176/90360 ( 0.2%)	1.03	57/122600 ( 0.0%)

5 of 66 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	79	PRO	CA-C	8.33	1.56	1.51	7	7
1	C	74	ALA	C-N	8.29	1.43	1.33	10	2
1	C	75	PRO	CA-C	8.26	1.56	1.51	2	3
1	A	170	PRO	CA-C	8.16	1.59	1.52	16	4
1	A	77	PRO	CA-C	8.08	1.56	1.51	8	2

5 of 35 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(°)	Ideal(°)	Models	
								Worst	Total
1	C	75	PRO	N-CA-C	7.46	119.80	110.70	10	2
1	A	183	HIS	CA-C-N	6.51	127.98	119.84	16	2
1	A	183	HIS	C-N-CA	6.51	127.98	119.84	16	2
1	C	183	HIS	CA-CB-CG	6.46	120.26	113.80	4	3
1	A	262	THR	CA-C-N	6.05	127.40	119.84	6	7

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	2120	2130	2127	14±3
1	C	2097	2107	2104	15±4
2	B	189	205	204	2±1
All	All	88120	88840	88700	558

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:118:ASP:HA	1:C:166:GLY:HA2	0.70	1.62	19	1
1:A:127:LEU:HB3	1:A:215:LEU:HD22	0.68	1.64	18	6
1:C:22:ILE:HD13	1:C:57:LEU:HB3	0.68	1.64	8	7
1:A:166:GLY:HA3	1:A:172:GLY:HA3	0.63	1.69	6	2
1:A:108:GLY:HA3	1:A:167:GLN:HB3	0.62	1.71	20	4

## 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	270/280 (96%)	233±4 (86±2%)	29±4 (11±1%)	9±2 (3±1%)	5	35
1	C	267/280 (95%)	235±3 (88±1%)	24±3 (9±1%)	8±2 (3±1%)	5	36
2	B	25/471 (5%)	14±3 (56±11%)	7±3 (28±11%)	4±2 (16±7%)	0	4
All	All	11240/20620 (55%)	9630 (86%)	1183 (11%)	427 (4%)	4	31

5 of 102 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	182	PRO	19
1	C	259	GLU	19
1	A	259	GLU	18
1	A	86	SER	16
1	C	80	PRO	16

### 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	218/224 (97%)	207±3 (95±1%)	11±3 (5±1%)	24	75
1	C	216/224 (96%)	203±4 (94±2%)	13±4 (6±2%)	19	68
2	B	18/359 (5%)	16±1 (91±6%)	2±1 (9±6%)	11	57
All	All	9040/16140 (56%)	8539 (94%)	501 (6%)	21	71

5 of 136 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	73	GLU	20
1	C	214	THR	20
1	C	73	GLU	19
1	A	95	GLU	17
1	C	95	GLU	14

### 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 oligosaccharides 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 23% for the well-defined parts and 20% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_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	1621
Number of shifts mapped to atoms	1621
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	225	$-0.11 \pm 0.11$	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	194	$0.20 \pm 0.08$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	86	$-0.16 \pm 0.06$	None needed (< 0.5 ppm)
$^{15}\text{N}$	218	$0.00 \pm 0.14$	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 20%, i.e. 1586 atoms were assigned a chemical shift out of a possible 7766. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	810/2773 (29%)	295/1134 (26%)	301/1130 (27%)	214/509 (42%)
Sidechain	776/4475 (17%)	432/2907 (15%)	344/1371 (25%)	0/197 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/518 (0%)	0/247 (0%)	0/254 (0%)	0/17 (0%)
Overall	1586/7766 (20%)	727/4288 (17%)	645/2755 (23%)	214/723 (30%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

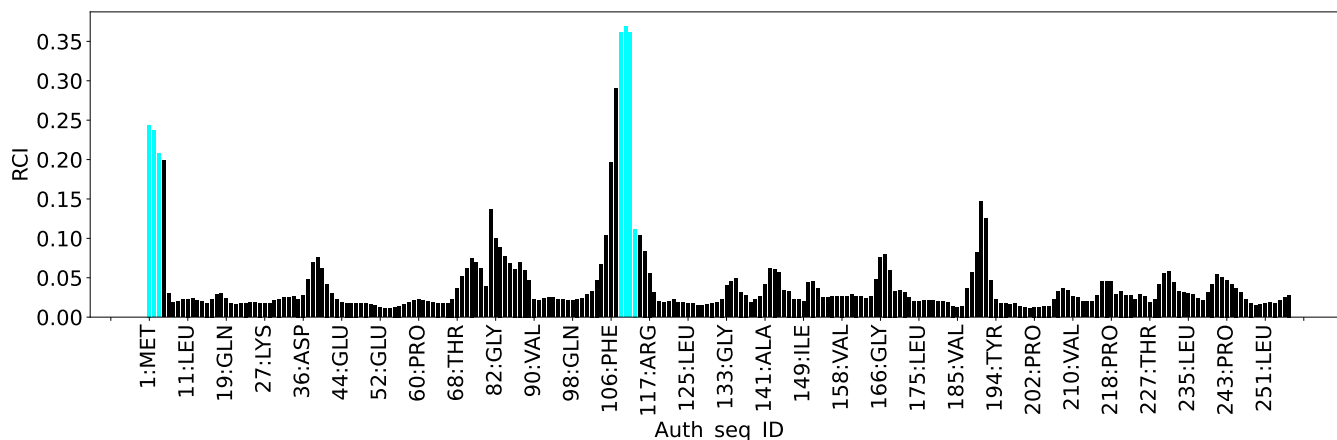
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	52	GLU	HA	2.21	2.24 – 6.23	-5.1
1	A	58	SER	HB2	2.59	2.61 – 5.13	-5.1

### 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\_shifts\_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	1105
Number of shifts mapped to atoms	1105
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 $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	31	$-0.18 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	32	$0.14 \pm 0.27$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	23	—	None (insufficient data)
$^{15}\text{N}$	379	$-0.80 \pm 0.14$	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 3%, i.e. 230 atoms were assigned a chemical shift out of a possible 7766. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	82/2773 (3%)	36/1134 (3%)	26/1130 (2%)	20/509 (4%)
Sidechain	136/4475 (3%)	95/2907 (3%)	40/1371 (3%)	1/197 (1%)
Aromatic	12/518 (2%)	6/247 (2%)	5/254 (2%)	1/17 (6%)
Overall	230/7766 (3%)	137/4288 (3%)	71/2755 (3%)	22/723 (3%)

### 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 B:

