Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	5XME
BMRB ID	:	36084
Title	:	Solution structure of C-terminal domain of TRADD
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Deposited on	:	2017-05-15

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:

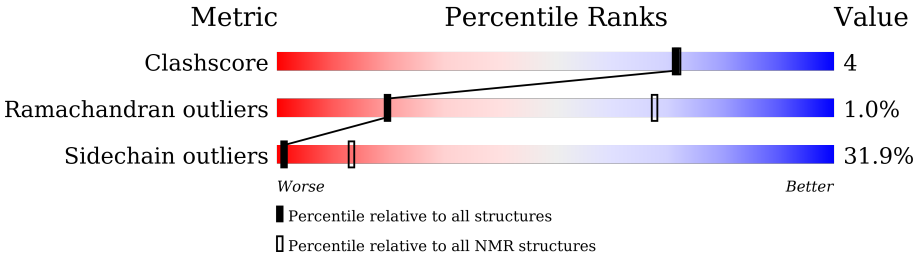
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 81%.

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	127	59% 24% 7% 10%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 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:202-A:306 (105)	0.29	3

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1827 atoms, of which 916 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor receptor type 1-associated DEATH domain protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	114	1827	570	916	170	170	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	MET	-	expression tag	UNP Q15628
A	187	HIS	-	expression tag	UNP Q15628
A	188	HIS	-	expression tag	UNP Q15628
A	189	HIS	-	expression tag	UNP Q15628
A	190	HIS	-	expression tag	UNP Q15628
A	191	HIS	-	expression tag	UNP Q15628
A	192	HIS	-	expression tag	UNP Q15628
A	193	SER	-	expression tag	UNP Q15628
A	194	SER	-	expression tag	UNP Q15628
A	195	GLY	-	expression tag	UNP Q15628
A	196	ARG	-	expression tag	UNP Q15628
A	197	GLY	-	expression tag	UNP Q15628
A	198	SER	-	expression tag	UNP Q15628

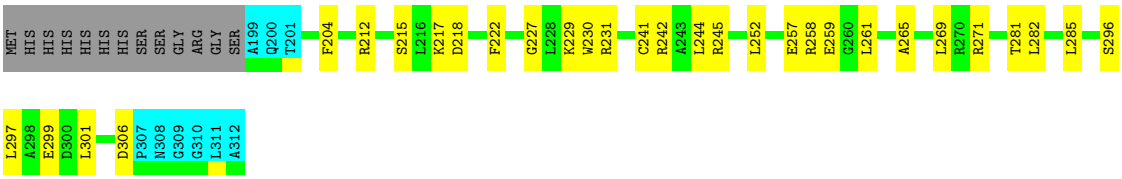
4 Residue-property plots (i)

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: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain A: 59% 24% 7% 10%



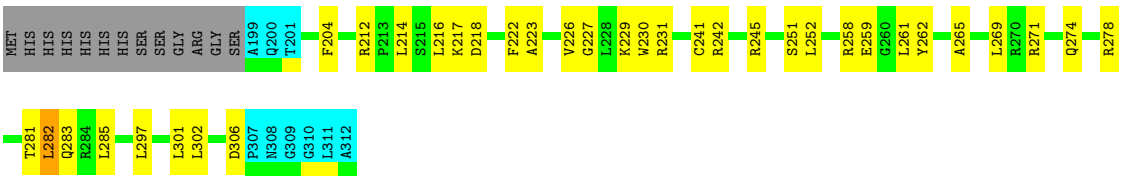
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

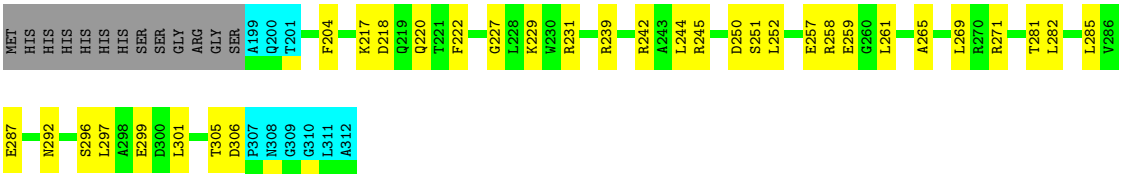
Chain A: 55% 27% • 7% 10%



4.2.2 Score per residue for model 2

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

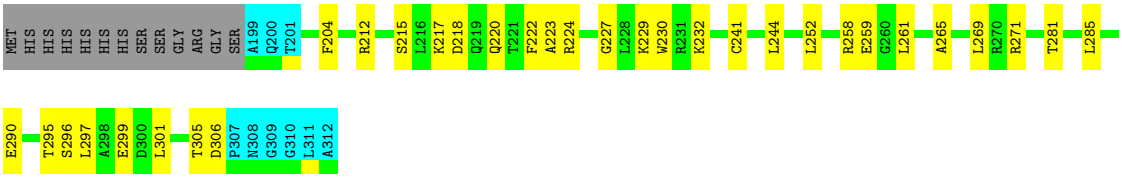
Chain A: 57% 26% 7% 10%



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

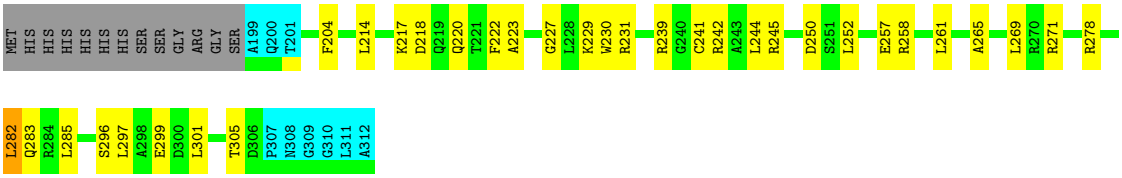
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

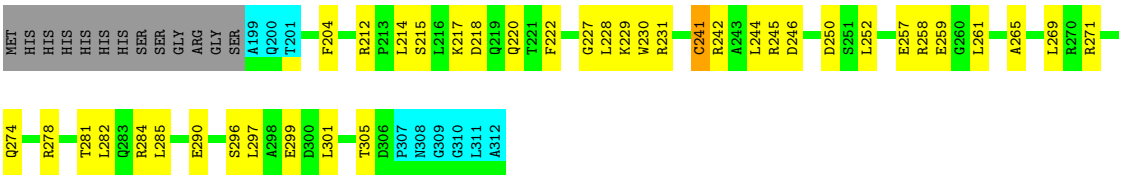
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain A: 53% 30% 7% 10%

MET HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLY SER A199 Q200 T201 F204 R212 S215 L216 K217 D218 Q219 Q220 T221 F222 G227 L228 K229 W230 R231 C241 R242 A243 L244 R245 D246 S251 L252 E257 R258 E259 G260 L261 A265 L269 R270 R271 R278 R279

A280 T281 L282 L285 E293 S296 L297 A298 E299 D300 L301 L304 P307 N308 G309 G310 L311 A312

4.2.7 Score per residue for model 7

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain A: 53% 30% 7% 10%

MET HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLY SER A199 Q200 T201 F204 L214 S215 L216 K217 D218 F222 A223 R224 G227 L228 K229 W230 R231 R239 G240 C241 D246 S251 L252 E257 R258 E259 G260 L261 A265 F266 Q267 L268 L269 R270 R271 Q274

L285 V286 E287 E290 E293 S296 L297 A298 E299 D300 L301 T305 D306 P307 N308 G309 G310 L311 A312

4.2.8 Score per residue for model 8

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain A: 52% 29% • 7% 10%

MET HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLY SER A199 Q200 T201 F204 R212 S215 L216 K217 D218 F222 G227 L228 K229 W230 R231 C241 R242 A243 L244 R245 D246 D250 S251 L252 E255 Y256 E257 R258 E259 G260 L261 A265 L269 R278 T281

L282 Q283 R284 L285 V286 E287 E290 E293 L294 T295 S296 L297 A298 E299 D300 L301 D306 P307 N308 G309 G310 L311 A312

4.2.9 Score per residue for model 9

• Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain A: 53% 29% • 7% 10%

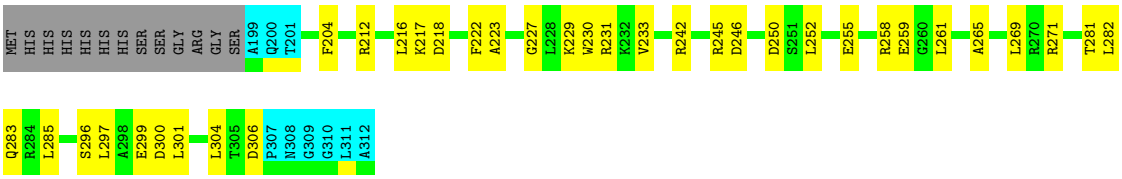
MET HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLY SER A199 Q200 T201 F204 R212 P213 L214 S215 L216 K217 D218 F222 A223 R224 G227 L228 K229 W230 R231 K232 V233 G234 R235 Q238 L244 R245 L252 E257 R258 L261 A265 L269 R270 R271 T281

L282 Q283 R284 L285 V286 E287 S296 L297 A298 E299 D300 L301 L304 T305 D306 P307 N308 G309 G310 L311 A312

4.2.10 Score per residue for model 10

- Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 10 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**
Amber	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	1
Total number of shifts	1320
Number of shifts mapped to atoms	1320
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	0.65±0.03	0±0/867 (0.0± 0.0%)	0.85±0.04	0±0/1169 (0.0± 0.0%)
All	All	0.65	0/8670 (0.0%)	0.85	1/11690 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	271	ARG	NE-CZ-NH2	5.07	122.83	120.30	6	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	854	862	862	6±1
All	All	8540	8620	8620	60

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:A:285:LEU:HD11	1:A:301:LEU:HD12	0.56	1.77	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:PHE:CE2	1:A:265:ALA:HB1	0.48	2.44	9	5
1:A:222:PHE:CE1	1:A:265:ALA:HB1	0.46	2.44	10	5
1:A:222:PHE:HA	1:A:301:LEU:HD22	0.45	1.88	5	9
1:A:230:TRP:HB2	1:A:265:ALA:HB2	0.44	1.88	9	9
1:A:285:LEU:HD11	1:A:301:LEU:CD1	0.44	2.42	1	1
1:A:223:ALA:CB	1:A:265:ALA:HB3	0.44	2.42	10	5
1:A:214:LEU:HD11	1:A:282:LEU:HD12	0.43	1.90	4	4
1:A:222:PHE:CE2	1:A:226:VAL:HG11	0.43	2.49	1	1
1:A:222:PHE:CZ	1:A:233:VAL:HG11	0.42	2.50	10	1
1:A:222:PHE:HA	1:A:301:LEU:HD21	0.42	1.91	1	1
1:A:285:LEU:HD13	1:A:285:LEU:C	0.42	2.35	5	5
1:A:241:CYS:HB3	1:A:244:LEU:HD12	0.41	1.93	8	2
1:A:222:PHE:CE1	1:A:233:VAL:HG11	0.41	2.50	9	1
1:A:223:ALA:HB2	1:A:265:ALA:HB3	0.41	1.93	3	1
1:A:214:LEU:N	1:A:214:LEU:HD12	0.40	2.31	7	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	105/127 (83%)	97±1 (92±1%)	7±1 (7±1%)	1±0 (1±0%)	20	68
All	All	1050/1270 (83%)	967 (92%)	72 (7%)	11 (1%)	20	68

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	227	GLY	10
1	A	280	ALA	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	89/105 (85%)	61±2 (68±3%)	28±2 (32±3%)	1 13
All	All	890/1050 (85%)	606 (68%)	284 (32%)	1 13

All 52 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	204	PHE	10
1	A	217	LYS	10
1	A	218	ASP	10
1	A	229	LYS	10
1	A	252	LEU	10
1	A	258	ARG	10
1	A	261	LEU	10
1	A	269	LEU	10
1	A	297	LEU	10
1	A	231	ARG	9
1	A	296	SER	9
1	A	299	GLU	9
1	A	245	ARG	8
1	A	259	GLU	8
1	A	271	ARG	8
1	A	281	THR	8
1	A	212	ARG	7
1	A	241	CYS	7
1	A	242	ARG	7
1	A	306	ASP	7
1	A	257	GLU	7
1	A	244	LEU	6
1	A	215	SER	6
1	A	251	SER	5
1	A	278	ARG	5
1	A	282	LEU	5
1	A	283	GLN	5
1	A	220	GLN	5
1	A	250	ASP	5
1	A	305	THR	5
1	A	246	ASP	5
1	A	216	LEU	4
1	A	287	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	290	GLU	4
1	A	300	ASP	4
1	A	274	GLN	3
1	A	239	ARG	3
1	A	224	ARG	3
1	A	228	LEU	3
1	A	293	GLU	3
1	A	304	LEU	3
1	A	295	THR	2
1	A	284	ARG	2
1	A	255	GLU	2
1	A	262	TYR	1
1	A	302	LEU	1
1	A	292	ASN	1
1	A	232	LYS	1
1	A	267	GLN	1
1	A	230	TRP	1
1	A	235	ARG	1
1	A	238	GLN	1

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 81% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ChemicalShifts.txt*

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	1320
Number of shifts mapped to atoms	1320
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	114	-0.04 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	105	0.26 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	110	0.49 ± 0.57	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 81%, i.e. 1236 atoms were assigned a chemical shift out of a possible 1521. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	421/526 (80%)	214/214 (100%)	105/210 (50%)	102/102 (100%)
Sidechain	761/906 (84%)	517/583 (89%)	231/270 (86%)	13/53 (25%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	54/89 (61%)	27/43 (63%)	26/45 (58%)	1/1 (100%)
Overall	1236/1521 (81%)	758/840 (90%)	362/525 (69%)	116/156 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1320 atoms were assigned a chemical shift out of a possible 1619. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	456/571 (80%)	232/233 (100%)	114/228 (50%)	110/110 (100%)
Sidechain	810/959 (84%)	551/618 (89%)	244/286 (85%)	15/55 (27%)
Aromatic	54/89 (61%)	27/43 (63%)	26/45 (58%)	1/1 (100%)
Overall	1320/1619 (82%)	810/894 (91%)	384/559 (69%)	126/166 (76%)

7.1.4 Statistically unusual chemical shifts (i)

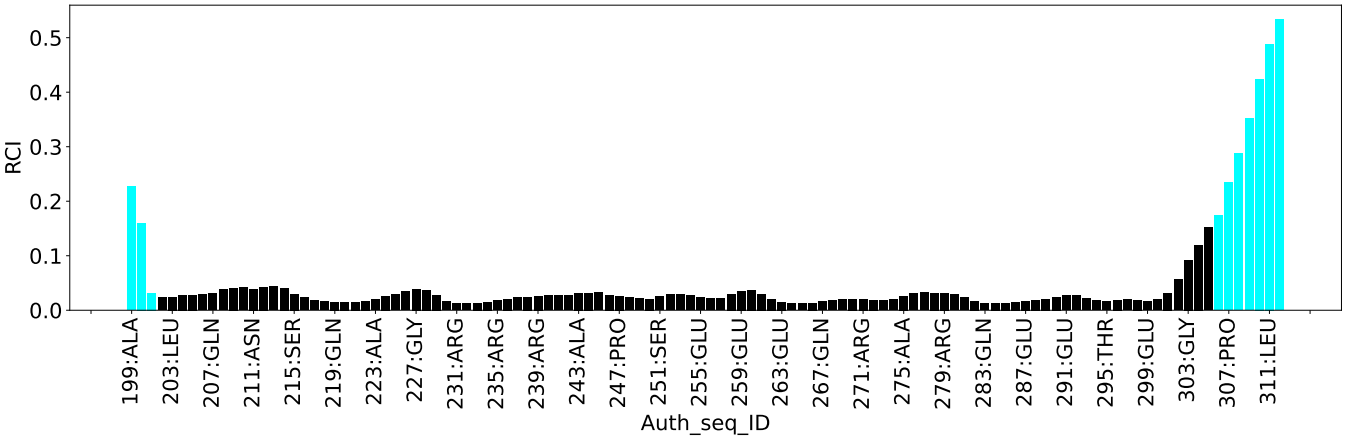
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	264	GLN	HB2	0.30	0.80 – 3.29	-7.0
1	A	267	GLN	HG3	0.43	0.91 – 3.68	-6.7

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
199:ALA
203:LEU
207:GLN
211:ASN
215:SER
219:GLN
223:ALA
227:GLY
231:ARG
235:ARG
239:ARG
243:ALA
247:PRO
251:SER
255:GLU
259:GLU
263:GLU
267:GLN
271:ARG
275:ALA
279:ARG
283:GLN
287:GLU
291:GLU
295:THR
299:GLU
303:GLY
307:PRO
311:LEU
Auth_seq_ID