Full wwPDB NMR Structure Validation Report (i)

Jun 15, 2024 – 11:28 AM EDT

PDB ID	:	2MAL
BMRB ID	:	19365
Title	:	Solution structure of Lipid Transfer Protein from Lentil Lens Culinaris
Authors	:	Gizatullina, A.K.; Mineev, K.S.; Shenkarev, Z.O.
Deposited on	:	2013-07-16

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:

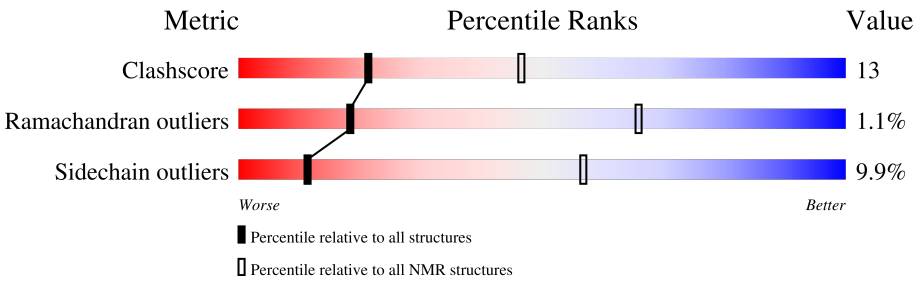
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 88%.

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	93	73% 18% • 5%

2 Ensemble composition and analysis (i)

This entry contains 20 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	A:1-A:88 (88)	0.52	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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1294 atoms, of which 651 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Non-specific lipid-transfer protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	93	1294	395	651	113	127	8	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: Non-specific lipid-transfer protein 2

Chain A: 73% 18% • 5%

A1 I2 S3 C4 V7 T8 L11 S12 P13 S25 C28 V32 L35 L36 T42 P43 A48 K53 L70 P71 V76 N77 I78 N89 T90 V91 K92 F93

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: Non-specific lipid-transfer protein 2

Chain A: 70% 23% • 5%

A1 I2 S3 C4 V7 T8 S9 D10 L11 S12 P13 S25 C28 V32 K33 K34 L35 T42 P43 Q46 A47 A48 L52 K53 L70 P71 V76 N77 I78 N89 T90 V91 K92 F93

4.2.2 Score per residue for model 2

• Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 76% 15% • 5%

A1 C4 V7 T8 L11 S12 P13 C28 V32 L35 L36 T42 P43 A48 L70 P71 I78 P79 Y80 N89 T90 V91 K92 F93

4.2.3 Score per residue for model 3

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 72% 20% • 5%

A1 I2 S3 C4 V7 S12 P13 C14 L15 C28 V32 L35 A38 A39 N40 T41 T42 P43 Q46 A47 A48 K53 I59 L70 P71 I78 N89 T90 V91 K92 F93

4.2.4 Score per residue for model 4

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 70% 23% • 5%

A1 I2 S3 C4 V7 T8 S9 D10 L11 S12 P13 S25 C28 V32 L35 T42 P43 D44 A48 K53 L70 P71 V76 N77 I78 P79 Y80 K81 N89 T90 V91 K92 F93

4.2.5 Score per residue for model 5

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 71% 22% • 5%

A1 I2 S3 C4 V7 T8 S9 D10 L11 S12 P13 S25 C28 V32 K33 K34 L35 T42 P43 A48 L52 K53 L70 P71 V76 N77 I78 N89 T90 V91 K92 F93

4.2.6 Score per residue for model 6

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 73% 19% • 5%

A1 I2 S3 C4 V7 T8 S9 D10 L11 S12 P13 S25 C28 V32 L35 T42 P43 A48 L52 L70 P71 G72 K73 I78 P79 Y80 N89 T90 V91 K92 F93

4.2.7 Score per residue for model 7

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 67% 25% • 5%

A1 I2 S3 C4 V7 T8 L11 S12 P13 C28 V32 L35 L36 N40 T41 T42 P43 D44 R45 A48 L52 A55 K61 L70 P71 I78 P79 Y80 K81 C88 N89 T90 V91 K92 F93

4.2.8 Score per residue for model 8

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 69% 22% • 5%

A1 I2 S3 C4 V7 T8 S9 D10 L11 S12 P13 S25 C28 V32 K33 K34 L35 L36 T42 P43 A48 K53 L70 P71 T78 P79 Y80 T86 N87 C88 N89 T90 V91 K92 F93

4.2.9 Score per residue for model 9

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 73% 18% • 5%

A1 I2 S3 C4 V7 T8 L11 S12 P13 S25 C28 V32 L35 L36 T42 P43 A48 A55 L70 P71 V76 N77 T78 N89 T90 V91 K92 F93

4.2.10 Score per residue for model 10

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 73% 19% • 5%

A1 I2 S3 C4 V7 T8 L11 S12 P13 S25 C28 V32 L35 T42 P43 A48 L52 K53 L70 P71 V76 N77 T78 N89 T90 V91 K92 F93

4.2.11 Score per residue for model 11

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 68% 24% • 5%

A1 I2 S3 C4 T8 S9 D10 L11 S12 P13 S25 C28 V32 K33 L36 T42 P43 A48 K53 L70 P71 V76 N77 T78 P79 Y80 K81 I82 N89 T90 V91 K92 F93

4.2.12 Score per residue for model 12

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 71% 19% • 5%

A1 I2 S3 C4 T8 S9 D10 L11 S12 P13 S25 C28 V32 L36 T42 P43 A48 K53 L70 P71 V76 N77 T78 I82 C88 N89 T90 V91 K92 F93

4.2.13 Score per residue for model 13

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 68% 22% 5% 5%

A1 C4 V7 T8 S9 D10 L11 S12 P13 S25 C28 V32 K33 K34 L35 L36 T42 P43 K61 L70 P71 V76 N77 I78 P79 Y80 K81 I82 N89 T90 V91 K92 F93

4.2.14 Score per residue for model 14

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 71% 20% • 5%

A1 C4 V7 T8 S9 D10 L11 S12 P13 C14 S25 V32 K33 K34 L35 L36 N40 T41 T42 P43 K53 L70 P71 V76 N77 I78 N89 T90 V91 K92 F93

4.2.15 Score per residue for model 15

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 71% 22% • 5%

A1 I2 S3 C4 V7 T8 S9 D10 L11 S12 P13 C28 V32 L35 T42 P43 A48 L52 K53 S58 K61 L70 P71 V76 N77 I78 N89 T90 V91 K92 F93

4.2.16 Score per residue for model 16

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 70% 22% • 5%

A1 C4 V7 T8 S9 D10 L11 S12 P13 S25 C28 V32 K33 K34 L35 L36 T42 P43 K53 L70 P71 V76 N77 I78 I82 N89 T90 V91 K92 F93

4.2.17 Score per residue for model 17

- Molecule 1: Non-specific lipid-transfer protein 2

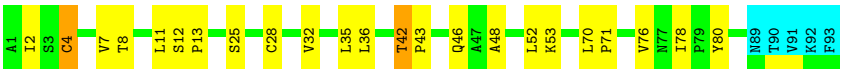
Chain A: 74% 17% • 5%

A1 I2 S3 C4 V7 S12 P13 C28 V32 L35 L36 T42 P43 A48 K53 L62 L70 P71 V76 N77 I78 S83 N89 T90 V91 K92 F93

4.2.18 Score per residue for model 18

- Molecule 1: Non-specific lipid-transfer protein 2

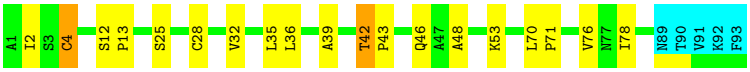
Chain A: 70% 23% • 5%



4.2.19 Score per residue for model 19

- Molecule 1: Non-specific lipid-transfer protein 2

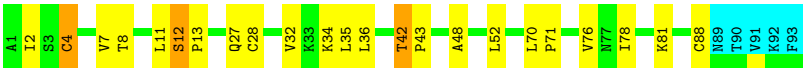
Chain A: 74% 18% • 5%



4.2.20 Score per residue for model 20

- Molecule 1: Non-specific lipid-transfer protein 2

Chain A: 70% 22% • 5%



5 Refinement protocol and experimental data overview (i)

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

Of the 200 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 solution	
TALOS	refinement	
Procheck	refinement	
CYANA	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	983
Number of shifts mapped to atoms	983
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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	A	601	607	609	16±2
All	All	12020	12140	12180	318

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:HG21	1:A:48:ALA:HB2	0.92	1.42	17	15
1:A:36:LEU:HD21	1:A:78:ILE:HG22	0.76	1.57	11	7
1:A:78:ILE:HD11	1:A:82:ILE:HD11	0.72	1.61	12	3
1:A:35:LEU:HD21	1:A:48:ALA:HB1	0.71	1.63	17	13
1:A:11:LEU:HD21	1:A:52:LEU:HD23	0.63	1.71	1	8
1:A:7:VAL:HG13	1:A:35:LEU:HD11	0.63	1.69	16	15
1:A:28:CYS:O	1:A:32:VAL:HG23	0.63	1.94	12	19
1:A:7:VAL:HG13	1:A:35:LEU:CD1	0.62	2.25	5	17
1:A:36:LEU:HD11	1:A:78:ILE:CG2	0.59	2.27	7	4
1:A:11:LEU:HD21	1:A:52:LEU:CD2	0.58	2.28	10	6
1:A:35:LEU:HD13	1:A:52:LEU:HD11	0.58	1.73	18	4
1:A:35:LEU:HD21	1:A:48:ALA:CB	0.58	2.27	19	10
1:A:62:LEU:HD21	1:A:83:SER:OG	0.57	2.00	17	1
1:A:36:LEU:HD11	1:A:78:ILE:HG22	0.56	1.76	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LEU:O	1:A:35:LEU:HD23	0.56	2.01	19	10
1:A:33:LYS:HG3	1:A:76:VAL:HG11	0.55	1.76	11	3
1:A:2:ILE:HD13	1:A:39:ALA:HB2	0.55	1.78	19	1
1:A:81:LYS:O	1:A:82:ILE:HD13	0.55	2.02	13	1
1:A:12:SER:N	1:A:13:PRO:HD2	0.55	2.17	20	20
1:A:36:LEU:HD12	1:A:76:VAL:HG21	0.55	1.79	20	3
1:A:36:LEU:HD21	1:A:78:ILE:CG2	0.54	2.31	11	2
1:A:42:THR:N	1:A:43:PRO:CD	0.52	2.73	4	20
1:A:8:THR:HA	1:A:11:LEU:HD12	0.52	1.81	14	15
1:A:32:VAL:HG21	1:A:70:LEU:HD11	0.51	1.80	14	1
1:A:36:LEU:HD12	1:A:76:VAL:CG2	0.51	2.36	16	3
1:A:70:LEU:N	1:A:71:PRO:HD2	0.50	2.22	12	20
1:A:2:ILE:HG21	1:A:48:ALA:CB	0.50	2.27	17	4
1:A:36:LEU:HD13	1:A:78:ILE:CG2	0.50	2.37	17	1
1:A:80:TYR:CD2	1:A:86:THR:HG23	0.49	2.42	8	1
1:A:7:VAL:HA	1:A:35:LEU:HD12	0.49	1.83	14	1
1:A:33:LYS:HA	1:A:76:VAL:HG21	0.47	1.86	11	1
1:A:40:ASN:OD1	1:A:41:THR:HG23	0.47	2.09	14	3
1:A:32:VAL:HG21	1:A:70:LEU:HD21	0.47	1.86	13	3
1:A:36:LEU:CD2	1:A:78:ILE:HG22	0.47	2.39	13	1
1:A:42:THR:N	1:A:43:PRO:HD2	0.45	2.27	3	20
1:A:2:ILE:CD1	1:A:39:ALA:HB2	0.45	2.41	19	1
1:A:12:SER:N	1:A:13:PRO:CD	0.44	2.80	20	2
1:A:14:CYS:SG	1:A:70:LEU:HD13	0.43	2.53	14	1
1:A:70:LEU:CB	1:A:71:PRO:CD	0.43	2.97	14	14
1:A:36:LEU:HD13	1:A:76:VAL:HG22	0.43	1.91	9	1
1:A:76:VAL:HG13	1:A:76:VAL:O	0.43	2.14	11	10
1:A:12:SER:CB	1:A:13:PRO:CD	0.43	2.97	14	18
1:A:11:LEU:HD13	1:A:55:ALA:CB	0.43	2.44	7	1
1:A:2:ILE:HD11	1:A:38:ALA:O	0.43	2.14	3	1
1:A:36:LEU:HD13	1:A:76:VAL:CG2	0.42	2.44	18	2
1:A:15:LEU:CD2	1:A:59:ILE:HD11	0.41	2.45	3	1
1:A:11:LEU:HD13	1:A:55:ALA:HB1	0.41	1.92	9	1
1:A:36:LEU:HD11	1:A:78:ILE:HG23	0.41	1.92	9	1
1:A:12:SER:HB3	1:A:13:PRO:HD3	0.41	1.92	12	1
1:A:35:LEU:C	1:A:35:LEU:HD23	0.41	2.36	14	1
1:A:42:THR:HB	1:A:43:PRO:HD3	0.40	1.93	13	1
1:A:35:LEU:HD23	1:A:35:LEU:O	0.40	2.15	6	1
1:A:70:LEU:N	1:A:71:PRO:CD	0.40	2.85	12	1
1:A:76:VAL:O	1:A:76:VAL:HG13	0.40	2.16	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	87/93 (94%)	82±1 (94±1%)	4±1 (5±1%)	1±0 (1±0%)	18	66
All	All	1740/1860 (94%)	1632 (94%)	88 (5%)	20 (1%)	18	66

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	4	CYS	20

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	67/72 (93%)	60±2 (90±3%)	7±2 (10±3%)	11	57
All	All	1340/1440 (93%)	1208 (90%)	132 (10%)	11	57

All 20 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	4	CYS	20
1	A	42	THR	20
1	A	78	ILE	20
1	A	25	SER	14
1	A	53	LYS	14
1	A	9	SER	8
1	A	34	LYS	7
1	A	81	LYS	5
1	A	10	ASP	5
1	A	77	ASN	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	46	GLN	3
1	A	61	LYS	3
1	A	12	SER	2
1	A	44	ASP	1
1	A	73	LYS	1
1	A	45	ARG	1
1	A	8	THR	1
1	A	36	LEU	1
1	A	58	SER	1
1	A	27	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 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_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	983
Number of shifts mapped to atoms	983
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	93	0.40 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	84	1.25 ± 0.10	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	85	0.30 ± 0.30	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 88%, i.e. 913 atoms were assigned a chemical shift out of a possible 1034. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	345/435 (79%)	177/178 (99%)	88/176 (50%)	80/81 (99%)
Sidechain	560/581 (96%)	382/384 (99%)	167/179 (93%)	11/18 (61%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	8/18 (44%)	8/8 (100%)	0/10 (0%)	0/0 (—%)
Overall	913/1034 (88%)	567/570 (99%)	255/365 (70%)	91/99 (92%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 975 atoms were assigned a chemical shift out of a possible 1108. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	365/460 (79%)	187/188 (99%)	93/186 (50%)	85/86 (99%)
Sidechain	597/620 (96%)	407/409 (100%)	178/191 (93%)	12/20 (60%)
Aromatic	13/28 (46%)	13/13 (100%)	0/15 (0%)	0/0 (—%)
Overall	975/1108 (88%)	607/610 (100%)	271/392 (69%)	97/106 (92%)

7.1.4 Statistically unusual chemical shifts (i)

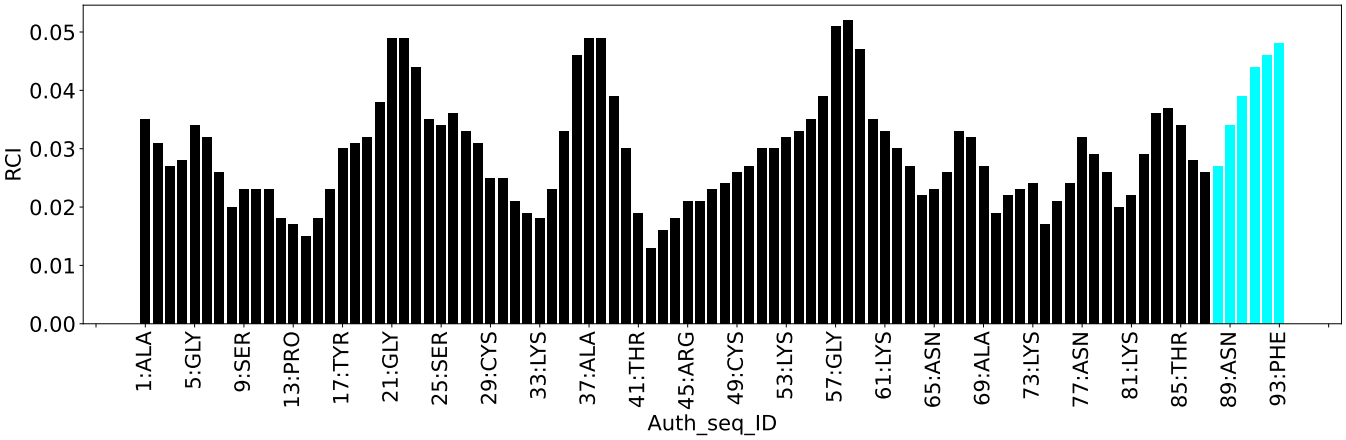
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	85	THR	HG1	5.01	0.08 – 2.19	18.4
1	A	16	THR	HG1	4.76	0.08 – 2.19	17.2
1	A	60	THR	HG1	4.75	0.08 – 2.19	17.1
1	A	34	LYS	CE	36.42	37.57 – 46.21	-6.3
1	A	53	LYS	CE	36.55	37.57 – 46.21	-6.2

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
0.00
0.01
0.02
0.03
0.04
0.05
1:ALA
5:GLY
9:SER
13:PRO
17:TYR
21:GLY
25:SER
29:CYS
33:LYS
37:ALA
41:THR
45:ARG
49:CYS
53:LYS
57:GLY
61:LYS
65:ASN
69:ALA
73:LYS
77:ASN
81:LYS
85:THR
89:ASN
93:PHE
Auth_seq_ID