



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:02 pm BST

PDB ID : 2LB6
Title : Structure of 18694Da MUP, typical to the major urinary protein family:
MUP9, MUP11, MUP15, MUP18 & MUP19
Authors : Phelan, M.M.; Mclean, L.; Beynon, R.J.; Hurst, J.L.; Lian, L.
Deposited on : 2011-03-23

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

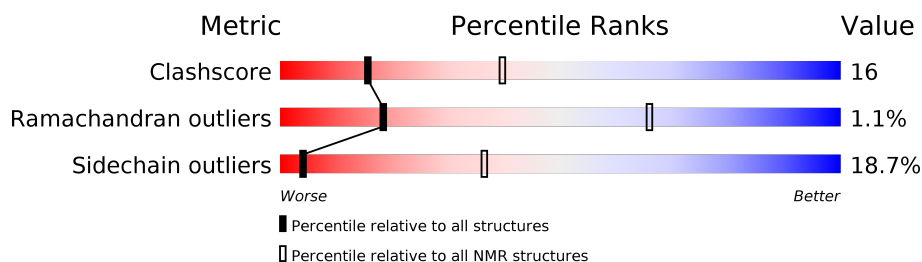
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	176	

2 Ensemble composition and analysis ⓘ

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

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:21-A:77, A:85-A:170 (143)	0.23	20

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 1 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2781 atoms, of which 1352 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major urinary protein 6.

Mol	Chain	Residues	Atoms						Trace
1	A	176	Total	C	H	N	O	S	0
			2781	885	1352	254	283	7	

There are 14 discrepancies between the modelled and reference sequences:

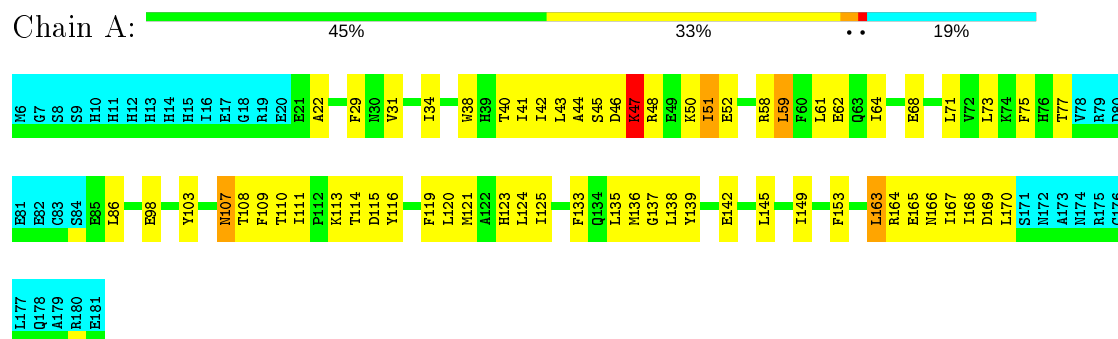
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	EXPRESSION TAG	UNP P02762
A	7	GLY	-	EXPRESSION TAG	UNP P02762
A	8	SER	-	EXPRESSION TAG	UNP P02762
A	9	SER	-	EXPRESSION TAG	UNP P02762
A	10	HIS	-	EXPRESSION TAG	UNP P02762
A	11	HIS	-	EXPRESSION TAG	UNP P02762
A	12	HIS	-	EXPRESSION TAG	UNP P02762
A	13	HIS	-	EXPRESSION TAG	UNP P02762
A	14	HIS	-	EXPRESSION TAG	UNP P02762
A	15	HIS	-	EXPRESSION TAG	UNP P02762
A	16	ILE	-	EXPRESSION TAG	UNP P02762
A	17	GLU	-	EXPRESSION TAG	UNP P02762
A	18	GLY	-	EXPRESSION TAG	UNP P02762
A	19	ARG	-	EXPRESSION TAG	UNP P02762

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Major urinary protein 6

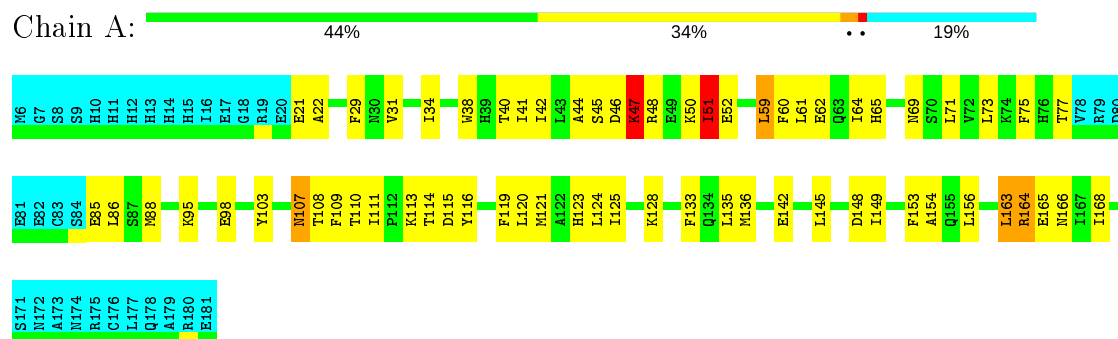


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

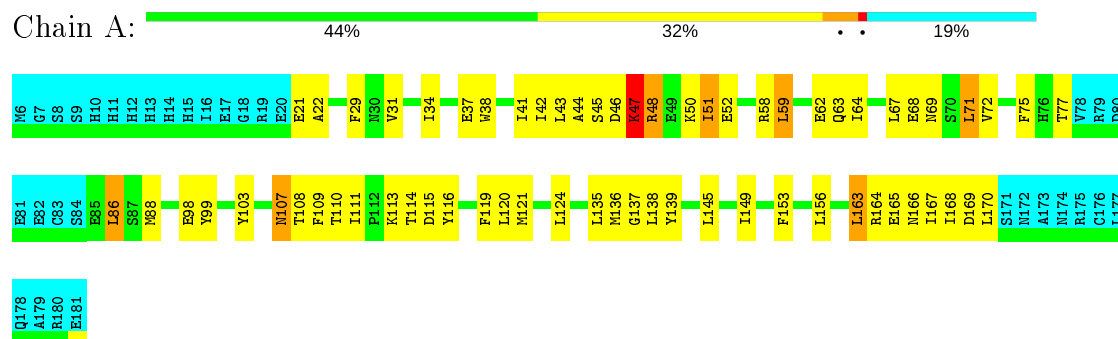
4.2.1 Score per residue for model 1

- Molecule 1: Major urinary protein 6



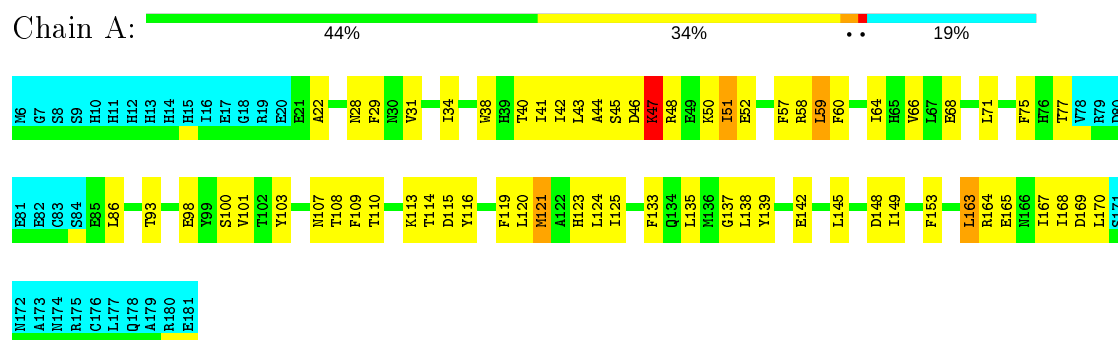
4.2.2 Score per residue for model 2

- Molecule 1: Major urinary protein 6



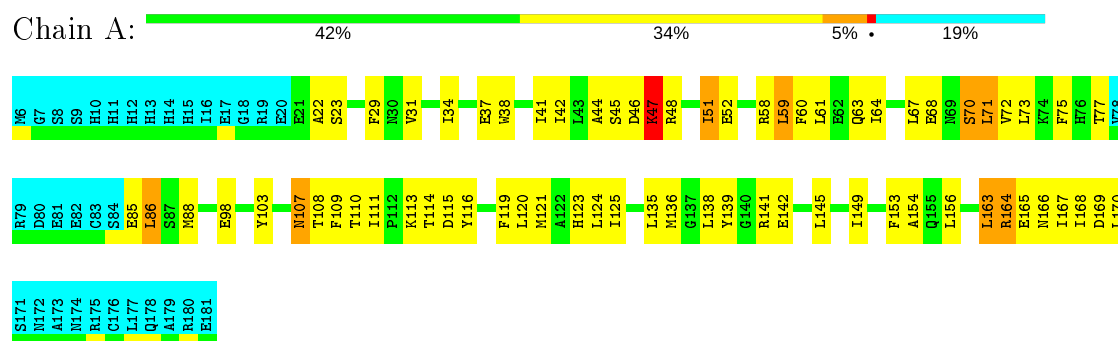
4.2.3 Score per residue for model 3

- Molecule 1: Major urinary protein 6



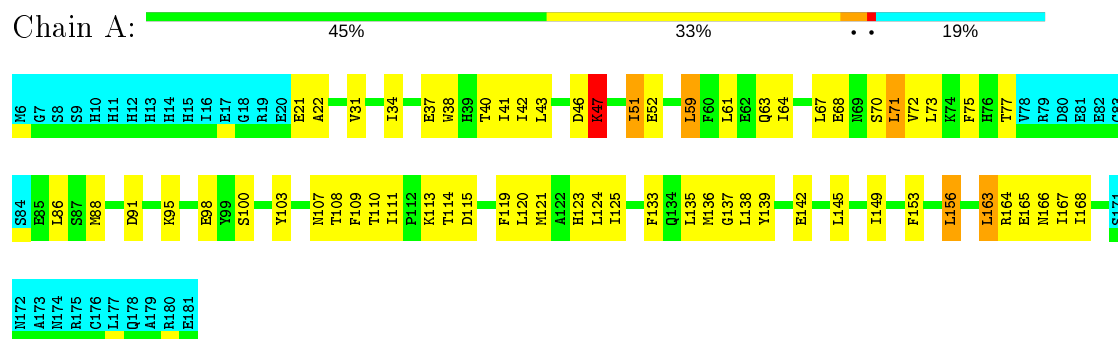
4.2.4 Score per residue for model 4

- Molecule 1: Major urinary protein 6



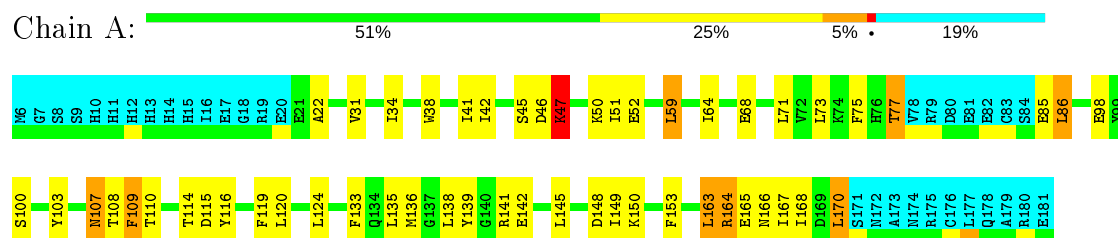
4.2.8 Score per residue for model 8

- Molecule 1: Major urinary protein 6



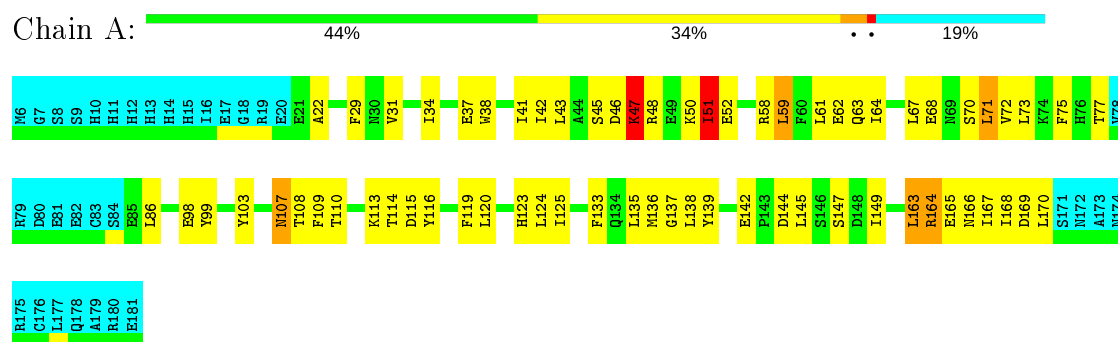
4.2.9 Score per residue for model 9

- Molecule 1: Major urinary protein 6



4.2.10 Score per residue for model 10

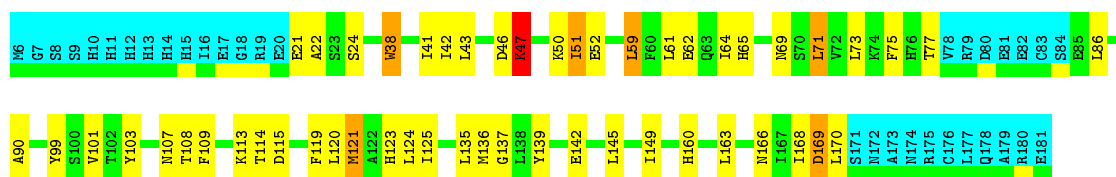
- Molecule 1: Major urinary protein 6



4.2.11 Score per residue for model 11

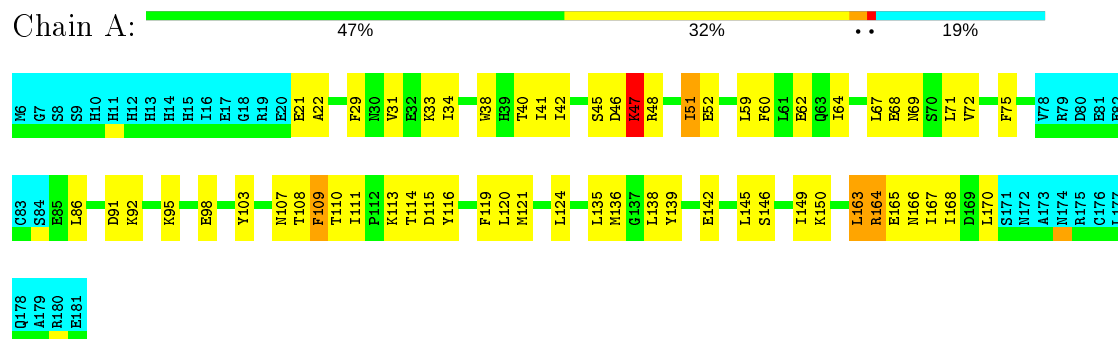
- Molecule 1: Major urinary protein 6





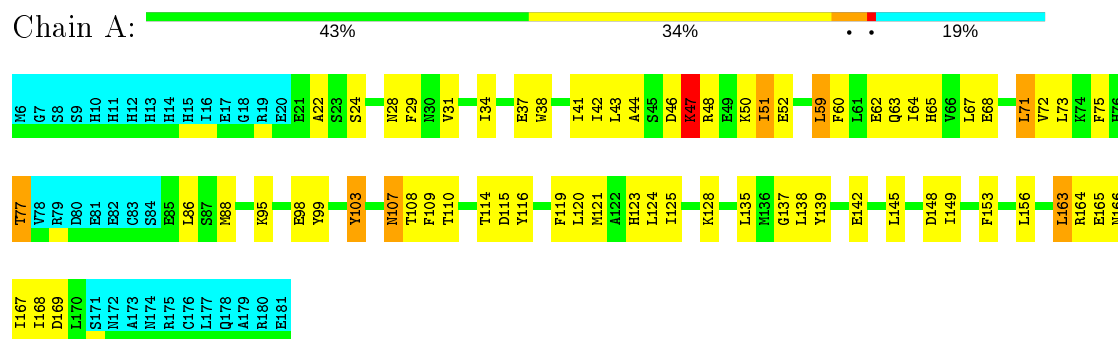
4.2.12 Score per residue for model 12

- Molecule 1: Major urinary protein 6



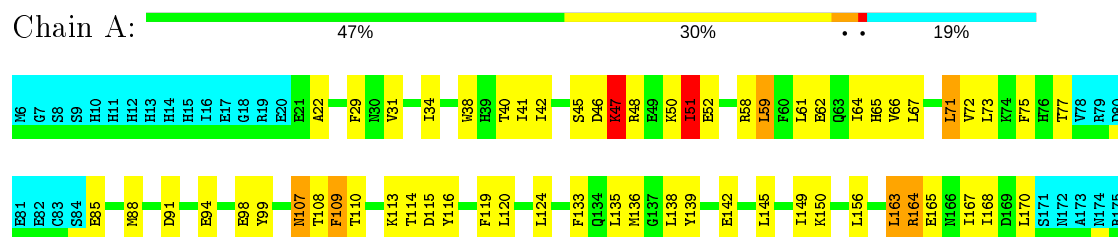
4.2.13 Score per residue for model 13

- Molecule 1: Major urinary protein 6



4.2.14 Score per residue for model 14

- Molecule 1: Major urinary protein 6



G176
L177
Q178
A179
R180
E181

4.2.15 Score per residue for model 15

- Molecule 1: Major urinary protein 6

Chain A: 47% 30% 19%

W6 G7 S8 S9 H10 H11 H12 H13 H14 H15 H16 I16 E17 G18 R19 E20 E21 A22 R27 N28 F29 V31 I34 W38 I41 I42 I43 I44 A44 S45 K47 I51 E52 L59 F60 L61 E62 Q63 I64 V66 L71 F75 H76 T77 V78 D80 E81 E82 C83 S84
E85 L86 S87 M88 V89 A90 Y99 Y103 N107 T108 F109 T110 T111 P112 K113 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 K128 F133 Q134 L135 M136 G137 L138 Y139 L145 I149 K150 F153 A154 L163 R164 E165 M166 I167 I168 D169 S171 M172 A173 M174

R175
C176
L177
Q178
A179
R180
E181

4.2.16 Score per residue for model 16

- Molecule 1: Major urinary protein 6

Chain A: 44% 33% 19%

W6 G7 S8 S9 H10 H11 H12 H13 H14 H15 H16 I16 E17 G18 R19 E20 E21 A22 S23 S24 R27 N28 V31 I34 W38 H39 T40 I41 I42 I43 L43 S45 D46 R48 E49 I51 E52 L59 F60 L61 I64 L67 E68 L71 V72 L73 F74 F75 H76 T77 V78
R79 D80 E81 E82 C83 S84 E85 L86 E98 Y103 D104 N107 T108 F109 T110 I111 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 L135 M136 G137 L138 Y139 G140 R141 L145 D148 I149 A154 L163 R164 E165 M166 I167 I168 S171 M172 A173 M174 C176

L177
Q178
A179
R180
E181

4.2.17 Score per residue for model 17

- Molecule 1: Major urinary protein 6

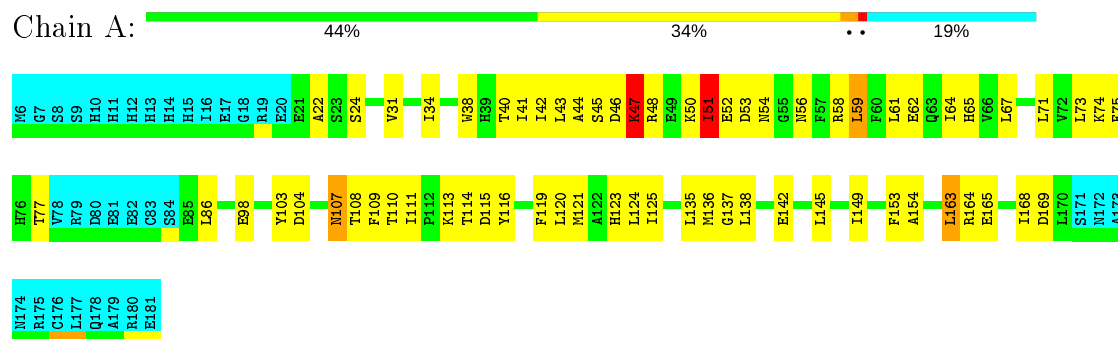
Chain A: 41% 37% 19%

W6 G7 S8 S9 H10 H11 H12 H13 H14 H15 H16 I16 E17 G18 R19 E20 E21 A22 S23 S24 R27 V31 E32 K33 I34 N35 W38 H39 T40 I41 I42 I43 A44 S45 D46 K47 I51 E52 F57 R58 L59 F60 L61 I64 I66 V66 L67 E68 L71 V72 L73 K74
F75 H76 T77 V78 R79 D80 E81 E82 C83 S84 E85 L86 S87 M88 K92 E98 S99 Y103 N107 T108 F109 T110 I111 P112 K113 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 N126 F133 Q134 L135 M136 G137 E142 L145 I149 K150 F153 A154

L163 R164 E165 M166 I167 I168 D169 L170 S171 M172 A173 M174 C176 L177 Q178 R180 E181

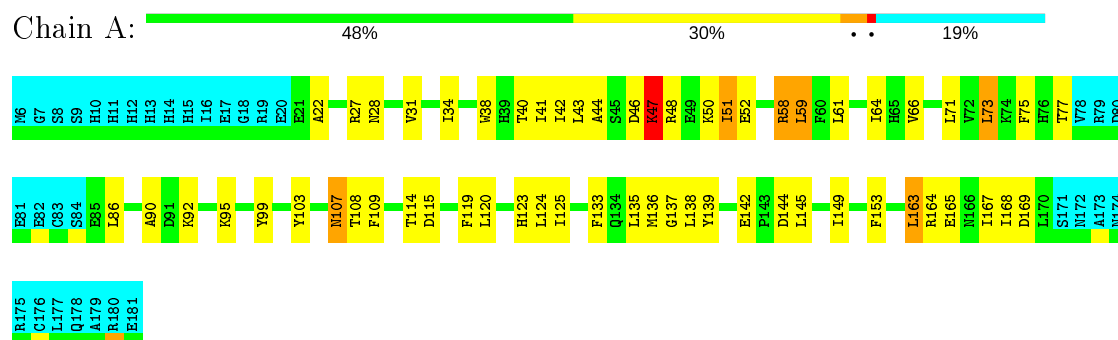
4.2.18 Score per residue for model 18

- Molecule 1: Major urinary protein 6



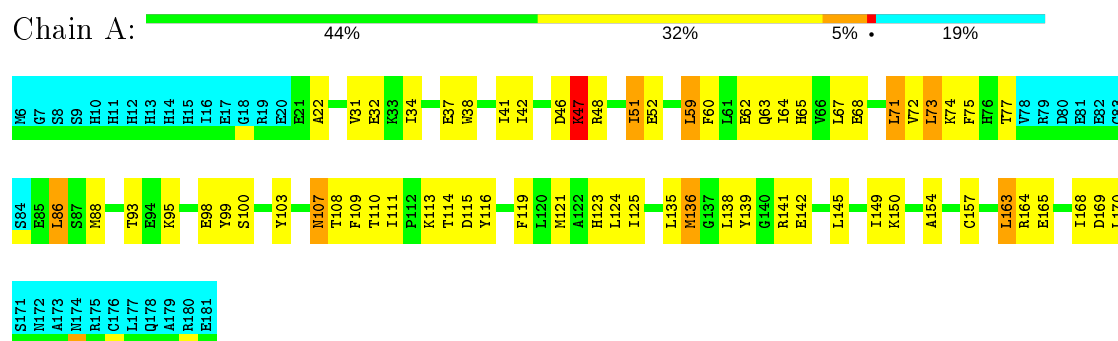
4.2.19 Score per residue for model 19

- Molecule 1: Major urinary protein 6



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Major urinary protein 6



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	2.1 and 3
CYANA	refinement	2.1 and 3

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1958
Number of shifts mapped to atoms	1958
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%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	1162	1120	1120	37±4
All	All	23240	22400	22400	745

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HG23	1:A:34:ILE:HD11	0.83	1.49	8	19
1:A:59:LEU:HD23	1:A:77:THR:HG23	0.80	1.52	16	2
1:A:38:TRP:CD1	1:A:64:ILE:HD12	0.73	2.19	3	20
1:A:41:ILE:HG21	1:A:145:LEU:HD12	0.72	1.62	4	20
1:A:170:LEU:HD22	1:A:170:LEU:O	0.68	1.87	9	1
1:A:51:ILE:HG13	1:A:168:ILE:HD13	0.66	1.67	14	14
1:A:73:LEU:HD12	1:A:75:PHE:CZ	0.66	2.26	20	15
1:A:59:LEU:HD23	1:A:77:THR:CG2	0.65	2.21	16	19
1:A:48:ARG:HD2	1:A:168:ILE:HD11	0.65	1.68	1	16
1:A:109:PHE:HB2	1:A:124:LEU:HD12	0.65	1.68	3	20
1:A:154:ALA:HB1	1:A:164:ARG:HD2	0.64	1.70	7	1
1:A:43:LEU:HD23	1:A:51:ILE:CG2	0.64	2.23	8	2
1:A:58:ARG:HG2	1:A:170:LEU:HD11	0.62	1.69	17	2
1:A:135:LEU:HD13	1:A:136:MET:N	0.62	2.09	9	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:HD13	1:A:121:MET:N	0.62	2.10	11	1
1:A:164:ARG:HA	1:A:167:ILE:HD13	0.62	1.72	14	11
1:A:58:ARG:CG	1:A:170:LEU:HD11	0.61	2.26	17	3
1:A:47:LYS:O	1:A:51:ILE:HD12	0.61	1.96	8	1
1:A:154:ALA:HB1	1:A:164:ARG:CD	0.61	2.25	4	4
1:A:59:LEU:HD22	1:A:75:PHE:HB3	0.61	1.73	16	11
1:A:107:ASN:OD1	1:A:124:LEU:HD11	0.60	1.97	19	15
1:A:67:LEU:HD11	1:A:72:VAL:CG2	0.60	2.26	12	2
1:A:22:ALA:O	1:A:114:THR:HG22	0.60	1.96	15	20
1:A:51:ILE:CG1	1:A:168:ILE:HD13	0.60	2.27	16	15
1:A:67:LEU:HD11	1:A:72:VAL:HG23	0.60	1.74	14	6
1:A:44:ALA:HB3	1:A:153:PHE:CZ	0.59	2.32	19	9
1:A:90:ALA:HB1	1:A:99:TYR:CB	0.59	2.28	19	1
1:A:123:HIS:CE1	1:A:125:ILE:HD11	0.58	2.32	6	15
1:A:154:ALA:HB1	1:A:164:ARG:HD3	0.58	1.75	18	7
1:A:86:LEU:HD12	1:A:88:MET:CE	0.58	2.29	17	5
1:A:45:SER:OG	1:A:135:LEU:HD22	0.57	1.99	5	1
1:A:38:TRP:HB3	1:A:61:LEU:HD23	0.57	1.77	4	11
1:A:59:LEU:HD22	1:A:75:PHE:CB	0.56	2.30	2	8
1:A:67:LEU:HD21	1:A:72:VAL:HG23	0.56	1.76	4	2
1:A:111:ILE:HG23	1:A:121:MET:O	0.56	2.01	18	13
1:A:109:PHE:CB	1:A:124:LEU:HD12	0.55	2.31	12	2
1:A:59:LEU:HD13	1:A:75:PHE:CD2	0.55	2.37	19	9
1:A:71:LEU:HD21	1:A:99:TYR:CE2	0.55	2.37	14	6
1:A:138:LEU:HD21	1:A:145:LEU:HD12	0.55	1.79	14	2
1:A:138:LEU:HD12	1:A:139:TYR:N	0.54	2.17	13	8
1:A:31:VAL:HG22	1:A:66:VAL:HG12	0.54	1.80	5	3
1:A:98:GLU:HA	1:A:110:THR:HG22	0.54	1.79	8	17
1:A:73:LEU:HD12	1:A:75:PHE:CE1	0.54	2.37	19	9
1:A:47:LYS:O	1:A:51:ILE:HD13	0.54	2.03	4	14
1:A:121:MET:CE	1:A:156:LEU:HD23	0.54	2.32	13	1
1:A:119:PHE:CD2	1:A:149:ILE:HG23	0.54	2.38	11	16
1:A:119:PHE:CD1	1:A:149:ILE:HG23	0.53	2.39	15	4
1:A:90:ALA:HB1	1:A:99:TYR:HB3	0.53	1.80	15	2
1:A:136:MET:SD	1:A:156:LEU:HD23	0.53	2.44	14	3
1:A:31:VAL:HG22	1:A:66:VAL:CG1	0.53	2.34	5	3
1:A:59:LEU:HD12	1:A:59:LEU:O	0.53	2.03	12	1
1:A:156:LEU:HD23	1:A:156:LEU:O	0.53	2.04	1	1
1:A:48:ARG:CD	1:A:168:ILE:HD11	0.53	2.34	13	6
1:A:138:LEU:HD23	1:A:139:TYR:N	0.53	2.18	2	6
1:A:41:ILE:HG21	1:A:145:LEU:CD1	0.53	2.32	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:PHE:CD2	1:A:135:LEU:HD13	0.53	2.39	3	2
1:A:166:ASN:O	1:A:168:ILE:HD12	0.53	2.04	16	14
1:A:58:ARG:HG3	1:A:170:LEU:HD11	0.52	1.81	6	2
1:A:71:LEU:O	1:A:71:LEU:HD12	0.52	2.04	15	1
1:A:43:LEU:HD12	1:A:137:GLY:HA2	0.52	1.82	18	12
1:A:170:LEU:HD22	1:A:170:LEU:C	0.52	2.25	9	1
1:A:145:LEU:HD22	1:A:149:ILE:HG21	0.52	1.81	11	2
1:A:145:LEU:HD13	1:A:149:ILE:CG2	0.51	2.35	12	1
1:A:41:ILE:O	1:A:42:ILE:HD13	0.51	2.05	1	20
1:A:29:PHE:CD2	1:A:114:THR:HG21	0.51	2.40	3	9
1:A:138:LEU:HD22	1:A:153:PHE:HB2	0.51	1.81	9	4
1:A:86:LEU:HD12	1:A:88:MET:HE2	0.51	1.81	17	1
1:A:67:LEU:HD22	1:A:67:LEU:N	0.50	2.22	16	2
1:A:121:MET:HE2	1:A:138:LEU:HD13	0.50	1.83	3	1
1:A:114:THR:HA	1:A:120:LEU:HD12	0.50	1.84	7	16
1:A:77:THR:CG2	1:A:86:LEU:HD22	0.50	2.36	13	1
1:A:86:LEU:HD12	1:A:88:MET:SD	0.49	2.46	2	1
1:A:86:LEU:HD23	1:A:86:LEU:H	0.49	1.67	13	1
1:A:120:LEU:C	1:A:120:LEU:HD13	0.49	2.27	11	1
1:A:75:PHE:HB2	1:A:86:LEU:HD21	0.49	1.85	13	1
1:A:163:LEU:HD12	1:A:165:GLU:HB2	0.49	1.82	14	17
1:A:29:PHE:CD1	1:A:114:THR:HG21	0.49	2.42	7	2
1:A:99:TYR:O	1:A:108:THR:HG22	0.49	2.08	6	1
1:A:67:LEU:N	1:A:67:LEU:HD22	0.49	2.23	8	2
1:A:38:TRP:HD1	1:A:64:ILE:HD12	0.48	1.68	2	9
1:A:38:TRP:CZ2	1:A:120:LEU:HD22	0.48	2.42	19	15
1:A:44:ALA:HB2	1:A:167:ILE:HG13	0.48	1.86	16	4
1:A:42:ILE:HD12	1:A:169:ASP:HA	0.48	1.85	4	7
1:A:86:LEU:HD12	1:A:88:MET:HE3	0.48	1.85	5	1
1:A:121:MET:CE	1:A:156:LEU:HD22	0.48	2.38	4	2
1:A:42:ILE:HG23	1:A:169:ASP:HA	0.48	1.85	20	3
1:A:22:ALA:C	1:A:114:THR:HG22	0.47	2.30	6	3
1:A:59:LEU:HD23	1:A:77:THR:HG22	0.47	1.84	13	2
1:A:61:LEU:HD22	1:A:139:TYR:CE1	0.47	2.44	19	1
1:A:45:SER:HB2	1:A:135:LEU:HD22	0.47	1.87	14	3
1:A:70:SER:C	1:A:71:LEU:HD23	0.47	2.29	4	3
1:A:22:ALA:HB1	1:A:27:ARG:O	0.47	2.09	16	2
1:A:46:ASP:O	1:A:47:LYS:HB2	0.46	2.10	8	20
1:A:50:LYS:NZ	1:A:135:LEU:HD23	0.46	2.24	13	1
1:A:41:ILE:HG22	1:A:42:ILE:HG12	0.46	1.86	4	3
1:A:41:ILE:HG21	1:A:145:LEU:CG	0.46	2.40	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:LEU:O	1:A:170:LEU:HD12	0.46	2.10	11	1
1:A:37:GLU:N	1:A:63:GLN:HE21	0.46	2.08	13	6
1:A:136:MET:CE	1:A:156:LEU:HD23	0.46	2.41	2	1
1:A:31:VAL:HG22	1:A:66:VAL:HG22	0.46	1.88	19	4
1:A:145:LEU:HD13	1:A:149:ILE:HG22	0.45	1.88	12	3
1:A:120:LEU:HD12	1:A:139:TYR:CD2	0.45	2.46	11	1
1:A:50:LYS:HZ1	1:A:135:LEU:HD23	0.45	1.72	13	1
1:A:44:ALA:HB3	1:A:153:PHE:CE2	0.45	2.47	1	1
1:A:41:ILE:HG21	1:A:145:LEU:HB2	0.45	1.88	5	10
1:A:73:LEU:HD23	1:A:73:LEU:H	0.44	1.71	14	2
1:A:43:LEU:HD23	1:A:51:ILE:HG23	0.44	1.90	8	1
1:A:120:LEU:HD12	1:A:139:TYR:HD2	0.44	1.73	11	1
1:A:121:MET:HE1	1:A:156:LEU:HD23	0.44	1.87	13	1
1:A:123:HIS:NE2	1:A:125:ILE:HD11	0.44	2.28	6	1
1:A:90:ALA:CA	1:A:101:VAL:HG12	0.44	2.43	11	1
1:A:138:LEU:HD21	1:A:145:LEU:CD1	0.43	2.42	14	2
1:A:35:ASN:ND2	1:A:66:VAL:HG22	0.43	2.28	17	2
1:A:93:THR:HG21	1:A:100:SER:HB3	0.43	1.90	20	2
1:A:121:MET:CE	1:A:138:LEU:HD13	0.43	2.42	3	1
1:A:46:ASP:O	1:A:47:LYS:CB	0.43	2.66	5	17
1:A:35:ASN:CG	1:A:66:VAL:HG22	0.43	2.34	5	1
1:A:73:LEU:H	1:A:73:LEU:HD23	0.43	1.74	11	2
1:A:51:ILE:HG12	1:A:168:ILE:HD13	0.42	1.91	5	1
1:A:45:SER:OG	1:A:51:ILE:HD12	0.42	2.14	7	6
1:A:59:LEU:HD13	1:A:75:PHE:CD1	0.42	2.49	15	1
1:A:135:LEU:HD13	1:A:135:LEU:C	0.42	2.35	16	4
1:A:43:LEU:HD23	1:A:51:ILE:HG22	0.42	1.90	19	2
1:A:77:THR:HG22	1:A:86:LEU:HD22	0.42	1.92	13	1
1:A:124:LEU:C	1:A:124:LEU:HD23	0.41	2.35	3	2
1:A:59:LEU:HD13	1:A:75:PHE:HB3	0.41	1.92	12	1
1:A:73:LEU:N	1:A:73:LEU:HD23	0.41	2.30	20	1
1:A:88:MET:HE3	1:A:103:TYR:CD1	0.41	2.51	13	1
1:A:31:VAL:CG2	1:A:34:ILE:HD11	0.41	2.39	5	1
1:A:58:ARG:NE	1:A:170:LEU:HD11	0.41	2.29	7	1
1:A:73:LEU:HD23	1:A:73:LEU:N	0.41	2.31	10	1
1:A:59:LEU:HD13	1:A:75:PHE:HD2	0.41	1.76	11	1
1:A:86:LEU:N	1:A:86:LEU:HD23	0.40	2.31	9	1
1:A:58:ARG:CD	1:A:170:LEU:HD11	0.40	2.45	7	1
1:A:170:LEU:N	1:A:170:LEU:CD1	0.40	2.85	9	1
1:A:22:ALA:HB3	1:A:114:THR:CG2	0.40	2.47	12	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	143/176 (81%)	125±2 (88±1%)	16±2 (11±1%)	2±1 (1±0%)	18	66
All	All	2860/3520 (81%)	2508 (88%)	320 (11%)	32 (1%)	18	66

All 4 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	47	LYS	20
1	A	51	ILE	6
1	A	95	LYS	5
1	A	55	GLY	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	128/157 (82%)	104±3 (81±2%)	24±3 (19±2%)	4	36
All	All	2560/3140 (82%)	2081 (81%)	479 (19%)	4	36

All 67 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	107	ASN	20
1	A	108	THR	20
1	A	51	ILE	20
1	A	52	GLU	20
1	A	71	LEU	20
1	A	163	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	47	LYS	20
1	A	103	TYR	19
1	A	59	LEU	19
1	A	86	LEU	18
1	A	115	ASP	18
1	A	116	TYR	17
1	A	113	LYS	16
1	A	142	GLU	16
1	A	68	GLU	13
1	A	50	LYS	12
1	A	40	THR	12
1	A	62	GLU	11
1	A	133	PHE	11
1	A	60	PHE	9
1	A	21	GLU	9
1	A	24	SER	8
1	A	150	LYS	7
1	A	58	ARG	7
1	A	65	HIS	7
1	A	164	ARG	6
1	A	85	GLU	6
1	A	170	LEU	6
1	A	28	ASN	5
1	A	148	ASP	5
1	A	100	SER	5
1	A	141	ARG	4
1	A	27	ARG	4
1	A	91	ASP	4
1	A	74	LYS	4
1	A	69	ASN	4
1	A	92	LYS	3
1	A	109	PHE	3
1	A	169	ASP	3
1	A	95	LYS	3
1	A	128	LYS	3
1	A	88	MET	3
1	A	104	ASP	3
1	A	136	MET	3
1	A	23	SER	2
1	A	144	ASP	2
1	A	54	ASN	2
1	A	121	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	A	45	SER	2
1	A	101	VAL	2
1	A	77	THR	2
1	A	33	LYS	2
1	A	73	LEU	2
1	A	53	ASP	2
1	A	70	SER	1
1	A	56	ASN	1
1	A	147	SER	1
1	A	39	HIS	1
1	A	38	TRP	1
1	A	157	CYS	1
1	A	126	ASN	1
1	A	160	HIS	1
1	A	156	LEU	1
1	A	48	ARG	1
1	A	94	GLU	1
1	A	146	SER	1
1	A	32	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1958
Number of shifts mapped to atoms	1958
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	165	-0.41 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	155	0.06 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	165	0.31 ± 0.20	None needed (< 0.5 ppm)
^{15}N	162	0.15 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

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. 1579 atoms were assigned a chemical shift out of a possible 1793. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	709/711 (100%)	283/284 (100%)	285/286 (100%)	141/141 (100%)
Sidechain	765/922 (83%)	479/536 (89%)	280/346 (81%)	6/40 (15%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	105/160 (66%)	55/87 (63%)	50/67 (75%)	0/6 (0%)
Overall	1579/1793 (88%)	817/907 (90%)	615/699 (88%)	147/187 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1810 atoms were assigned a chemical shift out of a possible 2207. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	819/876 (93%)	327/350 (93%)	330/352 (94%)	162/174 (93%)
Sidechain	886/1129 (78%)	556/660 (84%)	322/414 (78%)	8/55 (15%)
Aromatic	105/202 (52%)	55/111 (50%)	50/79 (63%)	0/12 (0%)
Overall	1810/2207 (82%)	938/1121 (84%)	702/845 (83%)	170/241 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	138	LEU	HB3	-0.72	3.34 – -0.26	-6.3
1	A	24	SER	HB3	2.26	5.25 – 2.45	-5.7
1	A	126	ASN	HB2	1.07	4.36 – 1.26	-5.6
1	A	104	ASP	HB3	1.13	4.07 – 1.27	-5.5

7.1.5 Random Coil Index (RCI) plots ⓘ

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.

Random coil index (RCI) for chain A:

