Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 07:50 PM EDT

PDB ID	:	2LUI
BMRB ID	:	18522
Title	:	Structure of the PICK PDZ domain in complex with the DAT C-terminal
Authors	:	Erlendsson, S.; Rathje, M.; Heidarsson, P.O.; Poulsen, F.M.; Madsen, K.L.; Teilum, K.; Gether, U.
Deposited on	:	2012-06-14

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:

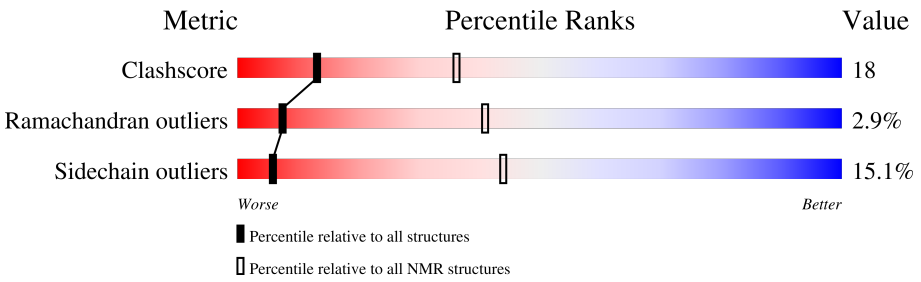
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 80%.

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	116	45% 21% 6% 28%

2 Ensemble composition and analysis (i)

This entry contains 20 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: *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:22-A:38, A:49-A:102, A:126-A:128 (74)	0.63	3
2	A:107-A:115 (9)	0.25	18

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 5 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1778 atoms, of which 904 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	116	1778	558	904	150	163	3	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP Q9EP80
A	14	SER	-	expression tag	UNP Q9EP80
A	15	PRO	-	expression tag	UNP Q9EP80
A	16	GLY	-	expression tag	UNP Q9EP80
A	17	ILE	-	expression tag	UNP Q9EP80
A	18	PRO	-	expression tag	UNP Q9EP80
A	111	LEU	-	SEE REMARK 999	UNP Q9EP80
A	112	GLU	-	SEE REMARK 999	UNP Q9EP80
A	113	VAL	-	SEE REMARK 999	UNP Q9EP80
A	114	LEU	-	SEE REMARK 999	UNP Q9EP80
A	115	PHE	-	SEE REMARK 999	UNP Q9EP80
A	116	GLN	-	SEE REMARK 999	UNP Q9EP80
A	117	GLY	-	SEE REMARK 999	UNP Q9EP80
A	118	PRO	-	SEE REMARK 999	UNP Q9EP80
A	119	GLN	-	SEE REMARK 999	UNP Q9EP80
A	120	PHE	-	SEE REMARK 999	UNP Q9EP80
A	121	THR	-	SEE REMARK 999	UNP Q9EP80
A	122	LEU	-	SEE REMARK 999	UNP Q9EP80
A	123	ARG	-	SEE REMARK 999	UNP Q9EP80
A	124	HIS	-	SEE REMARK 999	UNP Q9EP80
A	125	TRP	-	SEE REMARK 999	UNP Q9EP80
A	126	LEU	-	SEE REMARK 999	UNP Q9EP80
A	127	LYS	-	SEE REMARK 999	UNP Q9EP80
A	128	VAL	-	SEE REMARK 999	UNP Q9EP80

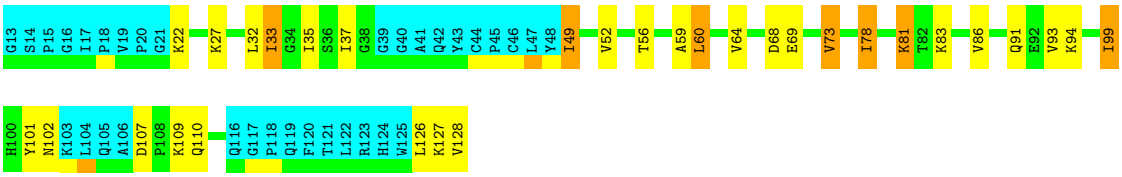
4 Residue-property plots (i)

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: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 45% 21% 6% 28%



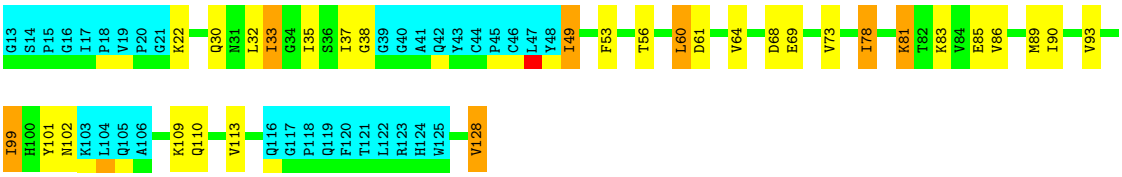
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

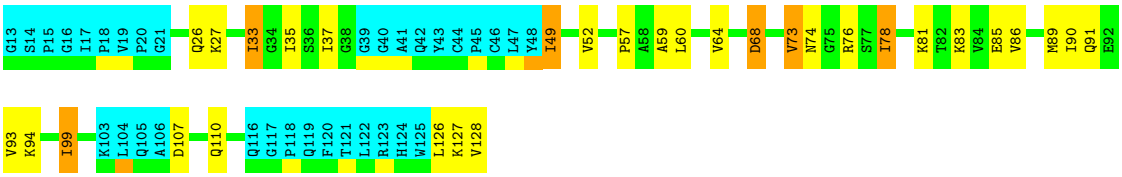
Chain A: 45% 21% 6% 28%



4.2.2 Score per residue for model 2

• Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

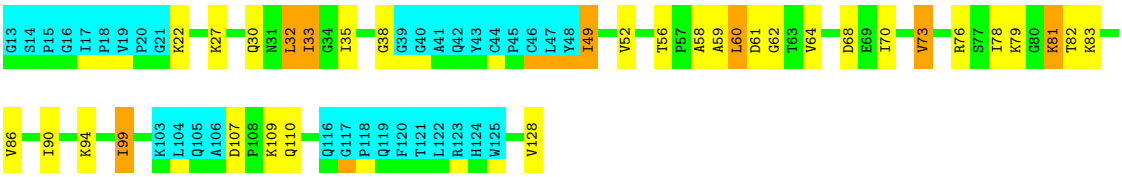
Chain A: 45% 22% 5% 28%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

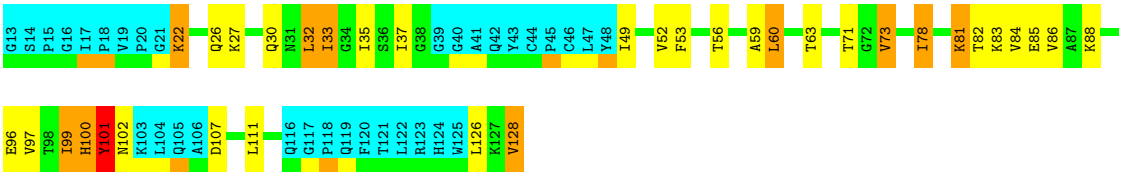
Chain A: 43% 22% 6% 28%



4.2.4 Score per residue for model 4

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

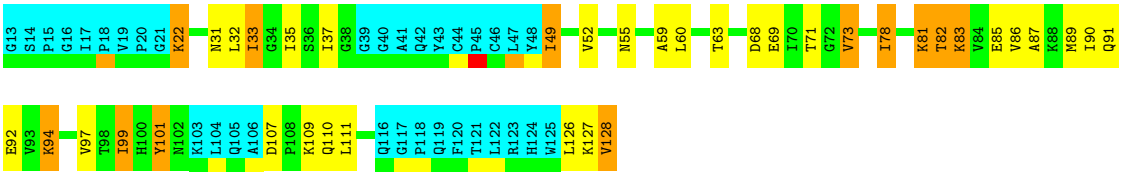
Chain A: 41% 21% 9% • 28%



4.2.5 Score per residue for model 5

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 39% 22% 10% 28%



4.2.6 Score per residue for model 6

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 46% 21% • • 28%

G13 S14 P15 G16 I17 P18 V19 P20 G21 Q26 K27 L32 I33 G34 I35 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 V50 Q51 T56 P57 A58 A59 L60 D61 G62 D68 E69 V73 I78 K81 T82 K83 V86 K94 G95 E96 V97 T98 I99

K103 L104 Q105 A106 K109 Q110 V113 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 L126 K127 V128

4.2.7 Score per residue for model 7

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 44% 20% 8% 28%

G13 S14 P15 G16 I17 P18 V19 P20 G21 K22 Q26 K27 Q30 N31 L32 I33 I37 G38 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 V52 T56 A59 L60 D61 E69 I70 V73 I78 K81 T82 K83 V86 N89 I90 Q91 E92 V93 K94

G95 E96 I99 K103 L104 Q105 A106 K109 Q110 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 L126 K127 V128

4.2.8 Score per residue for model 8

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 44% 19% 9% 28%

G13 S14 P15 G16 I17 P18 V19 P20 G21 K22 K27 Q30 N31 L32 I33 G34 I35 S36 I37 G38 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 V52 T56 P57 A58 A59 L60 D61 G62 T63 V64 D68 V73 R76 S77 I78 K81 T82 K83 V86

V93 I99 K103 L104 Q105 A106 D107 P108 E112 V113 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 L126 K127 V128

4.2.9 Score per residue for model 9

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 41% 23% 6% • 28%

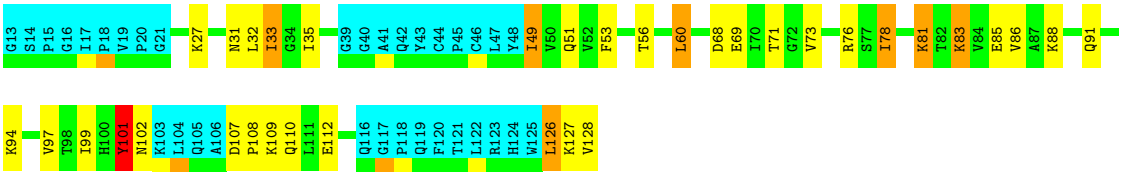
G13 S14 P15 G16 I17 P18 V19 P20 G21 K27 Q30 N31 L32 I33 G34 I35 S36 I37 G38 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 V50 Q51 V52 N55 A59 L60 D61 G62 T63 V64 D68 E69 I70 T71 G72 V73 I78 K81 T82 K83 V86 A87

I90 K94 I99 H100 Y101 N102 K103 L104 Q105 A106 L111 F115 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 L126 K127 V128

4.2.10 Score per residue for model 10

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

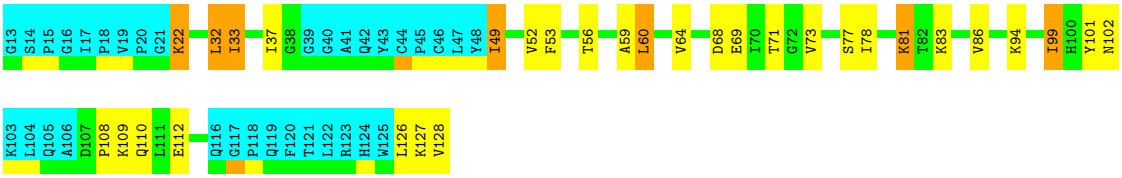
Chain A: 41% 23% 6% • 28%



4.2.11 Score per residue for model 11

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

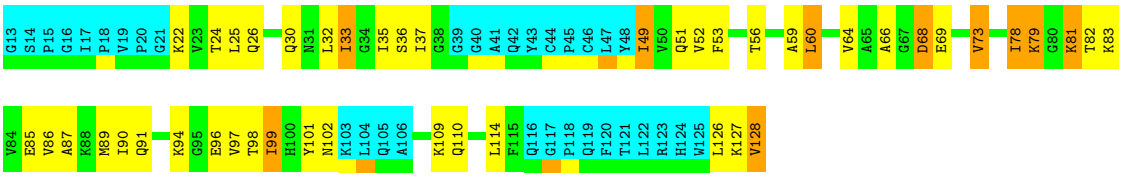
Chain A: 45% 21% 6% 28%



4.2.12 Score per residue for model 12

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

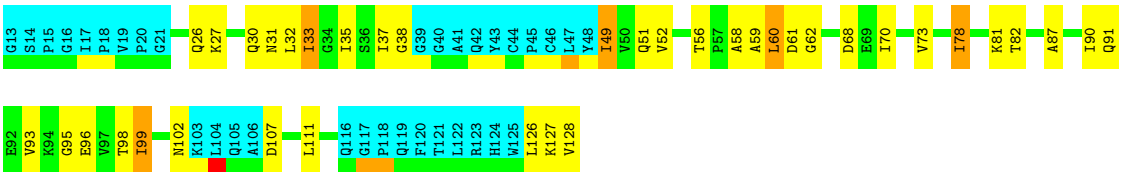
Chain A: 32% 31% 9% 28%



4.2.13 Score per residue for model 13

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 39% 28% • 28%



4.2.14 Score per residue for model 14

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 43% 20% 9% 28%

G13 S14 P15 G16 I17 P18 V19 P20 G21 K22 V23 T24 L25 Q26 K27 Q30 N31 L32 I33 S36 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 V52 T56 A59 L60 D61 G62 D68 V73 I78 K81 T82 K83 V86 A87 Q91 E92 V93

K94 G95 I99 N102 K103 L104 Q105 A106 K109 Q110 V113 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 L126 K127 V128

4.2.15 Score per residue for model 15

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 41% 21% 9% • 28%

G13 S14 P15 G16 I17 P18 V19 P20 G21 K27 L32 I33 I37 G38 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 V50 Q51 V52 T56 A59 L60 V64 D68 E69 I70 T71 G72 V73 N74 S77 I78 K81 T82 K83 V84 E85 V86 M89 I90 Q91

K94 T98 I99 H100 Y101 N102 K103 L104 Q105 A106 D107 P108 K109 Q110 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 V128

4.2.16 Score per residue for model 16

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 43% 19% 9% 28%

G13 S14 P15 G16 I17 P18 V19 P20 G21 K22 K27 L32 I33 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 F53 D54 N55 T56 A59 L60 D61 G62 T63 D68 V73 N74 I78 K81 T82 K83 V86 V93 V97 T98 I99 H100 Y101 N102

K103 L104 Q105 A106 D107 P108 K109 Q110 L111 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 L126 K127 V128

4.2.17 Score per residue for model 17

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 52% 15% 5% 28%

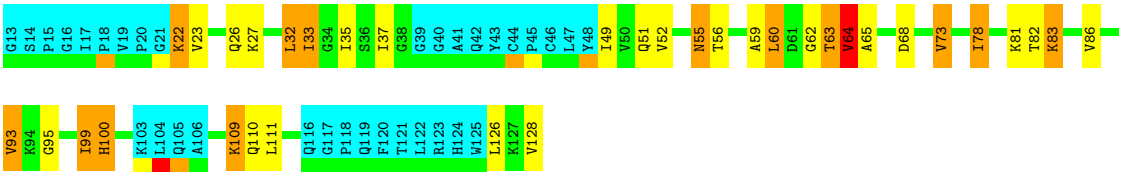
G13 S14 P15 G16 I17 P18 V19 P20 G21 Q30 N31 L32 I33 G39 G40 A41 Q42 Y43 C44 P45 C46 L47 Y48 I49 V52 F53 T56 A59 L60 D68 V73 I78 K79 G80 K81 T82 K83 V86 Q91 K94 I99 K103 L104 Q105 A106 D107 P108

K109 Q110 Q116 G117 P118 Q119 F120 T121 L122 R123 H124 W125 V128

4.2.18 Score per residue for model 18

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

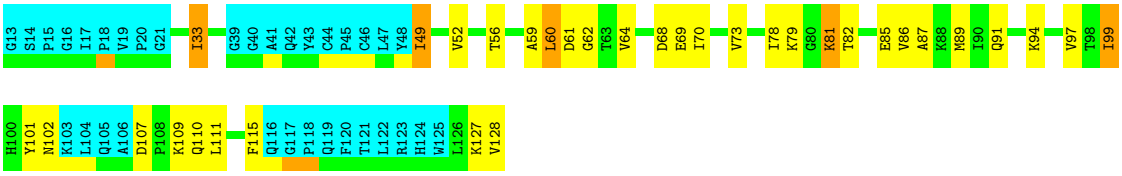
Chain A: 41% 18% 11% • 28%



4.2.19 Score per residue for model 19

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

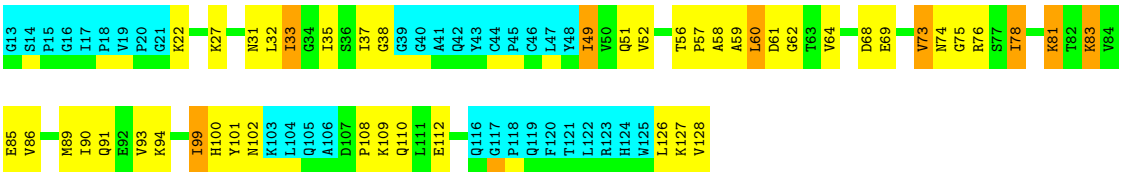
Chain A: 42% 25% • 28%



4.2.20 Score per residue for model 20

- Molecule 1: PICK1 PDZ DOMAIN FUSED TO THE C10 DAT LIGAND

Chain A: 32% 33% 7% 28%



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: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	
ARIA	refinement	
Analysis	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	1126
Number of shifts mapped to atoms	1126
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	626	661	660	24±5
All	All	12520	13220	13200	471

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD13	1:A:61:ASP:H	0.83	1.33	20	1
1:A:78:ILE:O	1:A:81:LYS:HE2	0.79	1.77	5	1
1:A:73:VAL:HG13	1:A:78:ILE:HG22	0.78	1.55	15	4
1:A:33:ILE:HG13	1:A:128:VAL:OXT	0.74	1.83	9	12
1:A:37:ILE:HG22	1:A:38:GLY:H	0.74	1.43	13	2
1:A:57:PRO:HA	1:A:60:LEU:CD1	0.73	2.14	20	1
1:A:126:LEU:HD13	1:A:127:LYS:N	0.67	2.04	5	4
1:A:60:LEU:HD22	1:A:61:ASP:N	0.66	2.04	20	1
1:A:70:ILE:HG12	1:A:101:TYR:CE1	0.64	2.27	19	1
1:A:33:ILE:HG13	1:A:128:VAL:O	0.63	1.93	11	7
1:A:37:ILE:HB	1:A:126:LEU:HD12	0.62	1.71	7	3
1:A:69:GLU:HB3	1:A:101:TYR:CD2	0.62	2.29	10	1
1:A:35:ILE:HD11	1:A:128:VAL:HG23	0.62	1.72	12	4
1:A:60:LEU:HD13	1:A:61:ASP:N	0.60	2.10	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ILE:HB	1:A:101:TYR:CE2	0.60	2.30	19	1
1:A:81:LYS:CG	1:A:86:VAL:HG13	0.60	2.26	19	1
1:A:81:LYS:HE3	1:A:81:LYS:C	0.60	2.17	5	1
1:A:49:ILE:HG22	1:A:68:ASP:O	0.60	1.97	18	17
1:A:32:LEU:HB2	1:A:128:VAL:C	0.60	2.17	8	9
1:A:71:THR:HB	1:A:101:TYR:CD2	0.60	2.32	10	1
1:A:32:LEU:HB2	1:A:128:VAL:OXT	0.59	1.97	6	3
1:A:69:GLU:HB2	1:A:102:ASN:OD1	0.59	1.97	15	1
1:A:73:VAL:O	1:A:76:ARG:HG2	0.59	1.97	2	5
1:A:68:ASP:HB3	1:A:101:TYR:CD1	0.59	2.33	19	1
1:A:71:THR:HG22	1:A:101:TYR:CB	0.58	2.28	15	4
1:A:69:GLU:O	1:A:101:TYR:HB3	0.58	1.97	10	4
1:A:73:VAL:HG12	1:A:78:ILE:HG22	0.58	1.75	4	7
1:A:60:LEU:HD12	1:A:61:ASP:N	0.57	2.14	7	9
1:A:33:ILE:HG23	1:A:97:VAL:HG11	0.57	1.74	5	4
1:A:58:ALA:O	1:A:62:GLY:HA3	0.57	2.00	20	5
1:A:37:ILE:O	1:A:126:LEU:HB3	0.57	1.99	9	1
1:A:71:THR:HG22	1:A:101:TYR:HA	0.57	1.76	10	2
1:A:26:GLN:HB2	1:A:95:GLY:O	0.56	2.00	13	3
1:A:87:ALA:O	1:A:91:GLN:HG3	0.56	1.99	12	2
1:A:73:VAL:CG1	1:A:78:ILE:HG23	0.56	2.30	12	1
1:A:78:ILE:HB	1:A:86:VAL:HG11	0.56	1.77	10	9
1:A:27:LYS:NZ	1:A:91:GLN:HA	0.56	2.17	15	3
1:A:37:ILE:HB	1:A:126:LEU:CD2	0.55	2.31	18	2
1:A:27:LYS:HZ2	1:A:91:GLN:HA	0.55	1.61	7	1
1:A:64:VAL:HG11	1:A:99:ILE:HG13	0.55	1.79	12	8
1:A:81:LYS:N	1:A:81:LYS:HD2	0.54	2.15	18	15
1:A:33:ILE:O	1:A:56:THR:HB	0.54	2.02	19	10
1:A:79:LYS:HD2	1:A:79:LYS:O	0.54	2.01	17	1
1:A:87:ALA:HB2	1:A:126:LEU:HD11	0.54	1.79	5	2
1:A:33:ILE:HD11	1:A:90:ILE:HG21	0.54	1.80	13	1
1:A:27:LYS:HE2	1:A:90:ILE:O	0.54	2.03	9	4
1:A:85:GLU:O	1:A:89:MET:HG3	0.54	2.02	19	4
1:A:37:ILE:HB	1:A:126:LEU:HD23	0.53	1.78	9	1
1:A:64:VAL:HB	1:A:101:TYR:OH	0.53	2.03	19	1
1:A:81:LYS:HG3	1:A:86:VAL:HG13	0.53	1.80	19	1
1:A:128:VAL:OXT	1:A:128:VAL:HG13	0.53	2.04	7	9
1:A:78:ILE:HD12	1:A:79:LYS:N	0.53	2.18	3	2
1:A:22:LYS:HA	1:A:99:ILE:O	0.53	2.04	14	7
1:A:93:VAL:O	1:A:93:VAL:HG23	0.53	2.04	8	5
1:A:126:LEU:HD23	1:A:127:LYS:N	0.52	2.19	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HD11	1:A:90:ILE:HD13	0.52	1.81	5	3
1:A:81:LYS:HE3	1:A:89:MET:SD	0.52	2.45	7	1
1:A:83:LYS:O	1:A:86:VAL:HG22	0.52	2.04	2	10
1:A:81:LYS:N	1:A:81:LYS:HD3	0.52	2.18	19	1
1:A:108:PRO:O	1:A:112:GLU:HG2	0.52	2.04	10	4
1:A:51:GLN:HA	1:A:66:ALA:HB2	0.52	1.79	12	1
1:A:87:ALA:O	1:A:91:GLN:HG2	0.52	2.05	19	2
1:A:81:LYS:HG3	1:A:86:VAL:CG1	0.52	2.34	19	1
1:A:99:ILE:N	1:A:99:ILE:HD13	0.52	2.20	18	9
1:A:82:THR:O	1:A:86:VAL:HB	0.52	2.05	15	1
1:A:52:VAL:HG22	1:A:59:ALA:HB2	0.51	1.82	2	16
1:A:62:GLY:O	1:A:63:THR:HB	0.51	2.05	18	1
1:A:26:GLN:HA	1:A:96:GLU:HA	0.51	1.82	12	4
1:A:30:GLN:NE2	1:A:32:LEU:HD21	0.51	2.21	1	2
1:A:27:LYS:HG3	1:A:95:GLY:H	0.51	1.66	14	1
1:A:75:GLY:HA2	1:A:100:HIS:CD2	0.51	2.40	20	1
1:A:55:ASN:HA	1:A:60:LEU:HD23	0.51	1.82	18	1
1:A:60:LEU:CD1	1:A:61:ASP:H	0.50	2.14	20	1
1:A:30:GLN:HE21	1:A:32:LEU:HD21	0.50	1.67	1	2
1:A:73:VAL:HG12	1:A:78:ILE:HG23	0.50	1.84	3	2
1:A:69:GLU:HB3	1:A:102:ASN:O	0.50	2.07	19	1
1:A:64:VAL:HG12	1:A:101:TYR:CE1	0.50	2.41	12	1
1:A:73:VAL:HG11	1:A:86:VAL:HB	0.49	1.84	10	1
1:A:32:LEU:HD22	1:A:128:VAL:OXT	0.49	2.07	12	4
1:A:23:VAL:HG11	1:A:62:GLY:O	0.49	2.07	14	1
1:A:81:LYS:HE3	1:A:86:VAL:HG11	0.49	1.85	19	1
1:A:57:PRO:HA	1:A:60:LEU:HD11	0.49	1.84	20	1
1:A:85:GLU:O	1:A:89:MET:HG2	0.49	2.08	2	3
1:A:49:ILE:HB	1:A:70:ILE:HD13	0.49	1.84	3	1
1:A:81:LYS:HG2	1:A:82:THR:N	0.49	2.23	5	2
1:A:83:LYS:HA	1:A:86:VAL:HG22	0.49	1.85	5	6
1:A:100:HIS:O	1:A:101:TYR:HB2	0.48	2.09	4	2
1:A:27:LYS:HE2	1:A:31:ASN:C	0.48	2.28	13	2
1:A:83:LYS:HB3	1:A:126:LEU:HD22	0.48	1.85	12	2
1:A:37:ILE:HG22	1:A:38:GLY:N	0.48	2.17	13	2
1:A:52:VAL:HG11	1:A:65:ALA:HA	0.48	1.86	18	1
1:A:64:VAL:HA	1:A:101:TYR:OH	0.48	2.09	12	1
1:A:24:THR:HG22	1:A:98:THR:HG22	0.48	1.84	12	1
1:A:111:LEU:O	1:A:115:PHE:HB2	0.48	2.09	9	1
1:A:27:LYS:HE3	1:A:97:VAL:HG12	0.47	1.85	6	1
1:A:107:ASP:OD2	1:A:109:LYS:HG2	0.47	2.09	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:ASP:OD1	1:A:109:LYS:HG2	0.47	2.08	16	1
1:A:78:ILE:H	1:A:78:ILE:HD13	0.47	1.70	14	3
1:A:83:LYS:O	1:A:126:LEU:HD11	0.47	2.08	7	1
1:A:128:VAL:O	1:A:128:VAL:HG13	0.47	2.09	11	2
1:A:109:LYS:HG3	1:A:110:GLN:N	0.47	2.25	14	14
1:A:126:LEU:HG	1:A:127:LYS:N	0.47	2.24	12	2
1:A:93:VAL:HG23	1:A:94:LYS:N	0.47	2.25	7	1
1:A:107:ASP:H	1:A:110:GLN:CG	0.47	2.21	15	3
1:A:64:VAL:O	1:A:64:VAL:CG1	0.47	2.62	18	1
1:A:27:LYS:HZ3	1:A:91:GLN:HA	0.46	1.69	2	2
1:A:74:ASN:ND2	1:A:93:VAL:HG11	0.46	2.25	20	3
1:A:74:ASN:HA	1:A:98:THR:OG1	0.46	2.10	15	1
1:A:35:ILE:HG13	1:A:128:VAL:OXT	0.46	2.10	18	6
1:A:53:PHE:HB2	1:A:56:THR:CG2	0.46	2.41	17	7
1:A:82:THR:O	1:A:86:VAL:HG13	0.46	2.10	12	5
1:A:35:ILE:O	1:A:127:LYS:HA	0.46	2.10	8	1
1:A:37:ILE:HB	1:A:126:LEU:HD21	0.45	1.88	18	1
1:A:69:GLU:O	1:A:101:TYR:HA	0.45	2.10	11	2
1:A:81:LYS:CG	1:A:82:THR:N	0.45	2.78	19	1
1:A:128:VAL:OXT	1:A:128:VAL:HG22	0.45	2.12	6	2
1:A:36:SER:HA	1:A:127:LYS:HA	0.45	1.89	12	1
1:A:78:ILE:HD12	1:A:79:LYS:H	0.45	1.72	3	2
1:A:92:GLU:O	1:A:94:LYS:HG3	0.45	2.12	5	1
1:A:81:LYS:HG2	1:A:86:VAL:HG23	0.45	1.87	15	1
1:A:60:LEU:HG	1:A:61:ASP:H	0.45	1.72	3	6
1:A:32:LEU:HB2	1:A:128:VAL:O	0.45	2.12	10	4
1:A:62:GLY:O	1:A:63:THR:CB	0.45	2.65	18	1
1:A:22:LYS:HG2	1:A:22:LYS:O	0.45	2.12	5	1
1:A:71:THR:H	1:A:101:TYR:HB2	0.45	1.70	5	2
1:A:25:LEU:CD2	1:A:99:ILE:HD11	0.45	2.42	12	1
1:A:99:ILE:HD13	1:A:99:ILE:H	0.45	1.71	18	1
1:A:31:ASN:ND2	1:A:91:GLN:HB2	0.44	2.27	5	4
1:A:73:VAL:CG1	1:A:78:ILE:HG22	0.44	2.42	7	1
1:A:110:GLN:O	1:A:114:LEU:HG	0.44	2.13	12	1
1:A:71:THR:HG22	1:A:101:TYR:CA	0.44	2.42	10	2
1:A:71:THR:N	1:A:101:TYR:HB2	0.44	2.27	10	1
1:A:27:LYS:HD3	1:A:97:VAL:CG1	0.44	2.43	4	3
1:A:69:GLU:HB2	1:A:102:ASN:O	0.43	2.14	10	1
1:A:35:ILE:HD13	1:A:37:ILE:HG12	0.43	1.91	1	1
1:A:109:LYS:O	1:A:113:VAL:HG23	0.43	2.13	6	3
1:A:54:ASP:HA	1:A:59:ALA:CB	0.43	2.43	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:GLY:O	1:A:64:VAL:HG13	0.43	2.14	19	1
1:A:71:THR:HG22	1:A:101:TYR:CG	0.42	2.49	4	1
1:A:23:VAL:HG23	1:A:99:ILE:CG1	0.42	2.44	18	1
1:A:71:THR:HB	1:A:101:TYR:CG	0.42	2.49	10	1
1:A:81:LYS:HD3	1:A:81:LYS:C	0.42	2.34	19	1
1:A:37:ILE:HB	1:A:126:LEU:HD13	0.42	1.89	13	1
1:A:60:LEU:CG	1:A:61:ASP:H	0.42	2.28	7	6
1:A:107:ASP:O	1:A:111:LEU:N	0.42	2.53	16	5
1:A:26:GLN:O	1:A:57:PRO:HG3	0.42	2.15	2	1
1:A:49:ILE:HB	1:A:70:ILE:CG1	0.42	2.44	7	1
1:A:52:VAL:CG2	1:A:59:ALA:HB2	0.42	2.45	5	3
1:A:62:GLY:O	1:A:63:THR:HG22	0.42	2.15	9	1
1:A:25:LEU:HD21	1:A:62:GLY:HA2	0.42	1.92	14	1
1:A:60:LEU:CG	1:A:61:ASP:N	0.41	2.83	1	6
1:A:37:ILE:HB	1:A:126:LEU:HG	0.41	1.91	4	1
1:A:26:GLN:NE2	1:A:96:GLU:HA	0.41	2.30	7	1
1:A:35:ILE:HG22	1:A:52:VAL:HG23	0.41	1.91	20	2
1:A:56:THR:O	1:A:60:LEU:HD12	0.41	2.15	20	1
1:A:69:GLU:HB2	1:A:102:ASN:ND2	0.41	2.30	20	1
1:A:85:GLU:O	1:A:88:LYS:HB3	0.41	2.15	4	2
1:A:27:LYS:CE	1:A:97:VAL:HG12	0.41	2.45	6	1
1:A:23:VAL:HG23	1:A:99:ILE:HD11	0.41	1.92	18	1
1:A:101:TYR:CD1	1:A:102:ASN:HB2	0.41	2.51	4	1
1:A:99:ILE:HD13	1:A:99:ILE:N	0.41	2.31	7	1
1:A:83:LYS:CB	1:A:126:LEU:HG	0.41	2.46	16	1
1:A:26:GLN:HA	1:A:97:VAL:HG13	0.41	1.93	6	1
1:A:36:SER:HA	1:A:126:LEU:O	0.41	2.16	14	1
1:A:79:LYS:HE2	1:A:115:PHE:O	0.41	2.15	19	1
1:A:37:ILE:HB	1:A:126:LEU:CD1	0.41	2.44	7	1
1:A:27:LYS:HE2	1:A:31:ASN:O	0.41	2.16	8	1
1:A:71:THR:O	1:A:77:SER:HA	0.41	2.15	11	2
1:A:60:LEU:CD1	1:A:61:ASP:N	0.40	2.85	7	2
1:A:107:ASP:O	1:A:110:GLN:N	0.40	2.55	5	2
1:A:37:ILE:H	1:A:126:LEU:CB	0.40	2.29	7	1
1:A:81:LYS:HD2	1:A:81:LYS:N	0.40	2.32	15	1
1:A:87:ALA:HB2	1:A:126:LEU:CD1	0.40	2.46	9	1
1:A:35:ILE:HD11	1:A:128:VAL:HG12	0.40	1.92	6	1
1:A:27:LYS:CG	1:A:95:GLY:H	0.40	2.29	14	1
1:A:89:MET:O	1:A:93:VAL:HG13	0.40	2.17	20	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	82/116 (71%)	70±2 (86±2%)	9±2 (11±3%)	2±1 (3±2%)	7 41
All	All	1640/2320 (71%)	1404 (86%)	188 (11%)	48 (3%)	7 41

All 10 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	60	LEU	19
1	A	94	LYS	12
1	A	101	TYR	5
1	A	93	VAL	3
1	A	22	LYS	2
1	A	27	LYS	2
1	A	64	VAL	2
1	A	115	PHE	1
1	A	108	PRO	1
1	A	63	THR	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	69/94 (73%)	59±2 (85±3%)	10±2 (15±3%)	6 44
All	All	1380/1880 (73%)	1172 (85%)	208 (15%)	6 44

All 35 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	33	ILE	20
1	A	99	ILE	20
1	A	49	ILE	19
1	A	78	ILE	19
1	A	81	LYS	17
1	A	73	VAL	15
1	A	83	LYS	11
1	A	32	LEU	10
1	A	30	GLN	7
1	A	60	LEU	7
1	A	51	GLN	7
1	A	22	LYS	6
1	A	128	VAL	4
1	A	68	ASP	4
1	A	100	HIS	4
1	A	101	TYR	4
1	A	55	ASN	4
1	A	109	LYS	4
1	A	63	THR	3
1	A	98	THR	3
1	A	127	LYS	3
1	A	82	THR	2
1	A	126	LEU	2
1	A	79	LYS	2
1	A	84	VAL	1
1	A	27	LYS	1
1	A	69	GLU	1
1	A	31	ASN	1
1	A	102	ASN	1
1	A	93	VAL	1
1	A	74	ASN	1
1	A	86	VAL	1
1	A	91	GLN	1
1	A	107	ASP	1
1	A	64	VAL	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 80% 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_list*

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	1126
Number of shifts mapped to atoms	1126
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
$^{13}C_{\alpha}$	108	-0.02 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	92	0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	100	-0.02 ± 0.16	None needed (< 0.5 ppm)
^{15}N	98	0.37 ± 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 80%, i.e. 896 atoms were assigned a chemical shift out of a possible 1122. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	409/419 (98%)	167/172 (97%)	162/166 (98%)	80/81 (99%)
Sidechain	483/666 (73%)	339/435 (78%)	138/210 (66%)	6/21 (29%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	4/37 (11%)	4/18 (22%)	0/17 (0%)	0/2 (0%)
Overall	896/1122 (80%)	510/625 (82%)	300/393 (76%)	86/104 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1117 atoms were assigned a chemical shift out of a possible 1547. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	514/580 (89%)	208/239 (87%)	208/232 (90%)	98/109 (90%)
Sidechain	593/882 (67%)	412/577 (71%)	174/276 (63%)	7/29 (24%)
Aromatic	10/85 (12%)	9/41 (22%)	0/39 (0%)	1/5 (20%)
Overall	1117/1547 (72%)	629/857 (73%)	382/547 (70%)	106/143 (74%)

7.1.4 Statistically unusual chemical shifts (i)

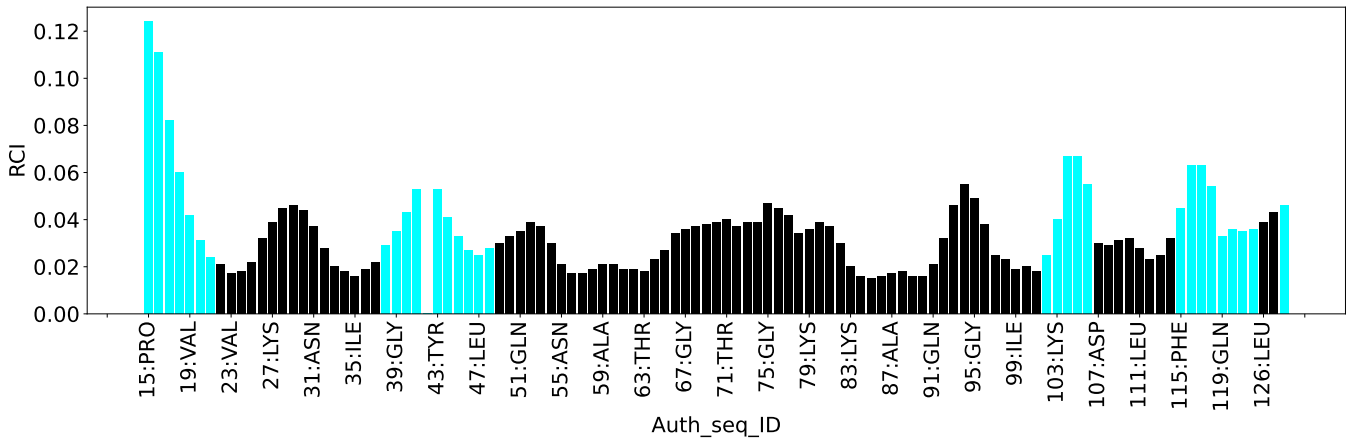
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	98	THR	HG1	5.19	0.08 – 2.19	19.2
1	A	56	THR	HG1	5.03	0.08 – 2.19	18.4

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
0.12
0.10
0.08
0.06
0.04
0.02
0.00
15:PRO
19:VAL
23:VAL
27:LYS
31:ASN
35:ILE
39:GLY
43:TYR
47:LEU
51:GLN
55:ASN
59:ALA
63:THR
67:GLY
71:THR
75:GLY
79:LYS
83:LYS
87:ALA
91:GLN
95:GLY
99:ILE
103:LYS
107:ASP
111:LEU
115:PHE
119:GLN
126:LEU
Auth_seq_ID