Full wwPDB NMR Structure Validation Report (i)

Feb 24, 2022 – 08:55 AM EST

PDB ID	:	1ZYI
Title	:	Solution structure of ICLN, a multifunctional protein involved in regulatory mechanisms as different as cell volume regulation and rna splicing
Authors	:	Fuerst, J.; Schedlbauer, A.; Gandini, R.; Garavaglia, M.L.; Siano, S.; Gschwentner, M.; Sarg, B.; Kontaxis, G.; Konrat, R.; Paulmichl, M.
Deposited on	:	2005-06-10

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

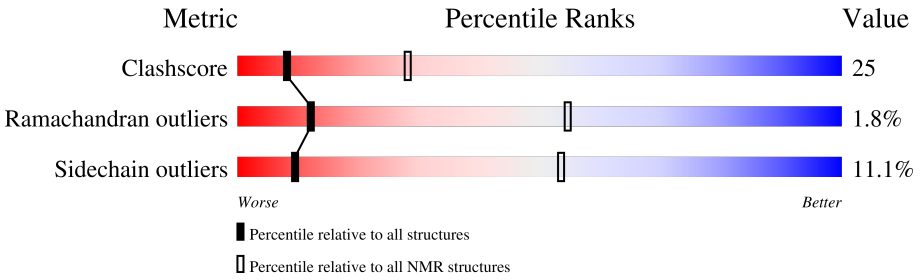
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 was not calculated.

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	171	27% 18% • 21% 32%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 11 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:28-A:65, A:71-A:75, A:85-A:93, A:115-A:142 (80)	0.48	11

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	1, 2, 3, 4, 5, 7, 8, 10, 11, 12, 13
2	9, 14
Single-model clusters	6; 15

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1742 atoms, of which 846 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Methylosome subunit pICln.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	116	1742	560	846	144	187	5	0

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P35521
A	2	HIS	-	expression tag	UNP P35521
A	3	HIS	-	expression tag	UNP P35521
A	4	HIS	-	expression tag	UNP P35521
A	5	HIS	-	expression tag	UNP P35521
A	6	HIS	-	expression tag	UNP P35521
A	7	HIS	-	expression tag	UNP P35521
A	8	LEU	-	expression tag	UNP P35521
A	9	GLU	-	expression tag	UNP P35521
A	10	MET	-	expression tag	UNP P35521
A	11	SER	-	expression tag	UNP P35521
A	12	PHE	-	expression tag	UNP P35521
A	13	LEU	-	expression tag	UNP P35521
A	14	LYS	-	expression tag	UNP P35521
A	15	SER	-	expression tag	UNP P35521
A	16	PHE	-	expression tag	UNP P35521
A	17	PRO	-	expression tag	UNP P35521
A	18	PRO	-	expression tag	UNP P35521
A	19	PRO	-	expression tag	UNP P35521
A	20	GLY	-	expression tag	UNP P35521
A	21	SER	-	expression tag	UNP P35521
A	22	ALA	-	expression tag	UNP P35521
A	23	GLU	-	expression tag	UNP P35521
A	24	GLY	-	expression tag	UNP P35521
A	25	LEU	-	expression tag	UNP P35521
A	26	ARG	-	expression tag	UNP P35521
A	143	HIS	-	cloning artifact	UNP P35521
A	144	PRO	-	cloning artifact	UNP P35521
A	145	ASP	-	cloning artifact	UNP P35521
A	146	PRO	-	cloning artifact	UNP P35521
A	147	GLU	-	cloning artifact	UNP P35521

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Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ASP	-	cloning artifact	UNP P35521
A	149	GLU	-	cloning artifact	UNP P35521
A	150	ASP	-	cloning artifact	UNP P35521
A	151	SER	-	cloning artifact	UNP P35521
A	152	ASP	-	cloning artifact	UNP P35521
A	153	ASP	-	cloning artifact	UNP P35521
A	154	TYR	-	cloning artifact	UNP P35521
A	155	ASP	-	cloning artifact	UNP P35521
A	156	GLY	-	cloning artifact	UNP P35521
A	157	GLU	-	cloning artifact	UNP P35521
A	158	GLU	-	cloning artifact	UNP P35521
A	159	TYR	-	cloning artifact	UNP P35521
A	160	ASP	-	cloning artifact	UNP P35521
A	161	VAL	-	cloning artifact	UNP P35521
A	162	GLU	-	cloning artifact	UNP P35521
A	163	ALA	-	cloning artifact	UNP P35521
A	164	HIS	-	cloning artifact	UNP P35521
A	165	GLU	-	cloning artifact	UNP P35521
A	166	GLN	-	cloning artifact	UNP P35521
A	167	GLY	-	cloning artifact	UNP P35521
A	168	GLN	-	cloning artifact	UNP P35521
A	169	GLU	-	cloning artifact	UNP P35521
A	170	ASN	-	cloning artifact	UNP P35521
A	171	ASP	-	cloning artifact	UNP P35521

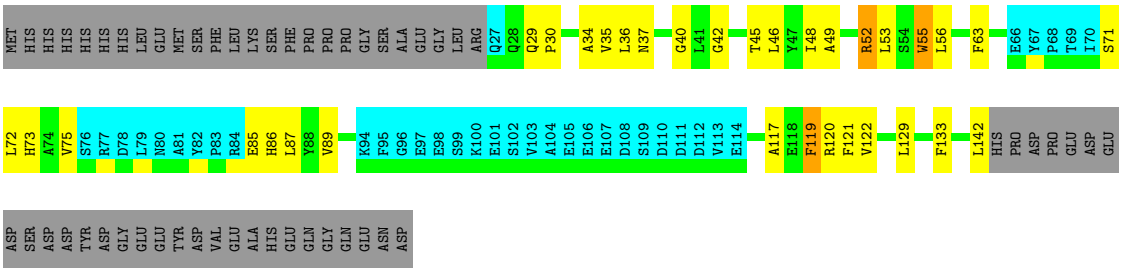
4 Residue-property plots (i)

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: Methylosome subunit pICln

Chain A: 27% 18% • 21% 32%



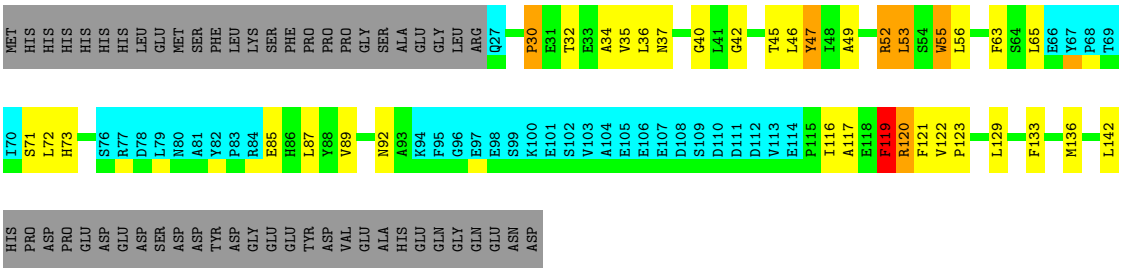
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Methylosome subunit pICln

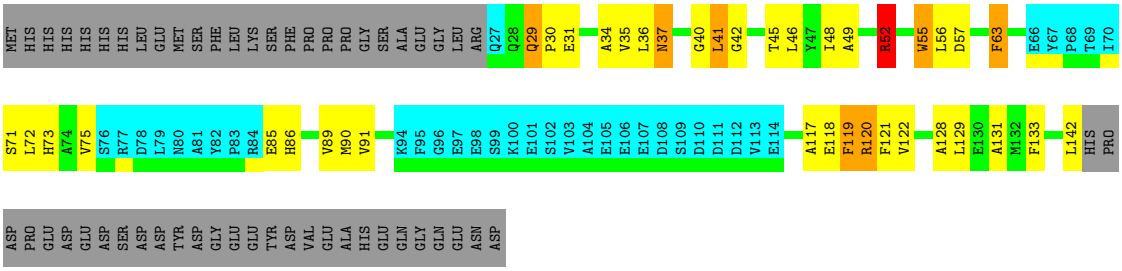
Chain A: 26% 17% • • 21% 32%



4.2.2 Score per residue for model 2

- Molecule 1: Methylosome subunit pICln

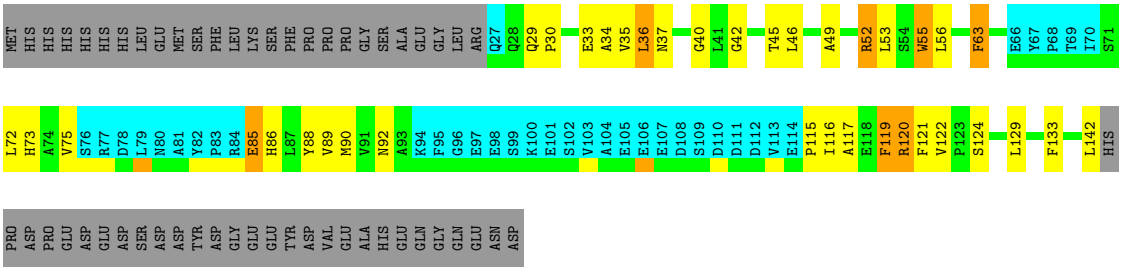
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Methylosome subunit pICln

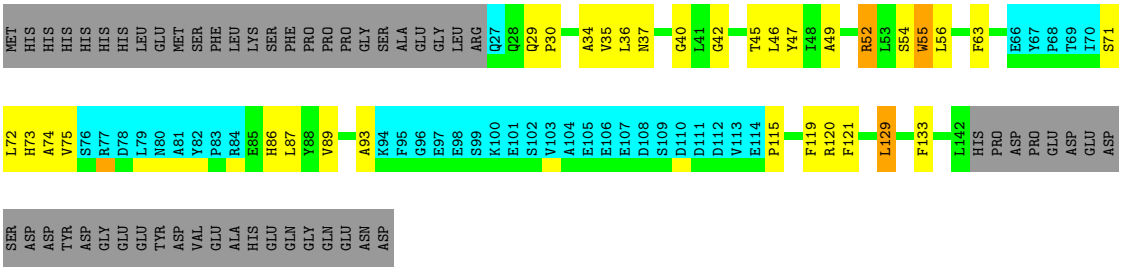
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Methylosome subunit pICln

Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Methylosome subunit pICln

Chain A: 26% 19% • 21% 32%

MET HIS HIS HIS HIS HIS HIS LEU GLU MET SER PHE LEU LYS SER PHE PRO PRO PRO GLY SER ALA GLU GLY LEU ARG Q27 P30 A34 V35 L36 K39 G42 T45 L46 Y47 I48 R52 L53 S54 W55 L56 E66 Y67 P68 T69 I70 S71 L72 H73 A74 V75 S76

R77 D78 L79 N80 A81 Y82 P83 R84 E85 H86 L87 Y88 V89 M90 V91 N92 A93 K94 F95 G96 E97 E98 S99 K100 E101 S102 V103 A104 E105 E106 E107 D108 S109 D110 D111 D112 V113 E114 P115 I116 F119 R120 F121 V122 D125 L129 M132 F133 T134 A135 E138 L142 HIS PRO

ASP PRO GLU ASP GLU ASP SER ASP ASP TYR ASP GLY GLU GLU TYR ASP VAL GLU ALA HIS GLU GLN GLY GLN GLU ASN ASP

4.2.6 Score per residue for model 6

• Molecule 1: Methylosome subunit pICln

Chain A: 32% 13% • 21% 32%

MET HIS HIS HIS HIS HIS HIS LEU GLU MET SER PHE LEU LYS SER PHE PRO PRO PRO GLY SER ALA GLU GLY LEU ARG Q27 P30 E33 A34 V35 L36 G40 L41 G42 T43 L46 Y47 I48 A49 R52 L53 S54 W55 L56 E66 Y67 P68 T69 I70 S71 L72 S76

R77 D78 L79 N80 A81 Y82 P83 R84 E85 H86 L87 Y88 V89 K94 F95 G96 E97 E98 S99 K100 E101 S102 V103 A104 E105 E106 E107 D108 S109 D110 D111 D112 V113 E114 F119 R120 F121 L129 A135 M136 L142 HIS PRO ASP PRO GLU ASP GLU ASP SER ASP ASP TYR ASP GLY

GLU GLU TYR ASP VAL GLU ALA HIS GLU GLN GLY GLN GLU ASN ASP

4.2.7 Score per residue for model 7

• Molecule 1: Methylosome subunit pICln

Chain A: 29% 16% • 21% 32%

MET HIS HIS HIS HIS HIS HIS LEU GLU MET SER PHE LEU LYS SER PHE PRO PRO PRO GLY SER ALA GLU GLY LEU ARG Q27 P30 A34 V35 L36 N37 G40 L41 G42 T45 L46 Y47 I48 R52 W55 L56 F63 E66 Y67 P68 T69 I70 S71 L72 H73 A74

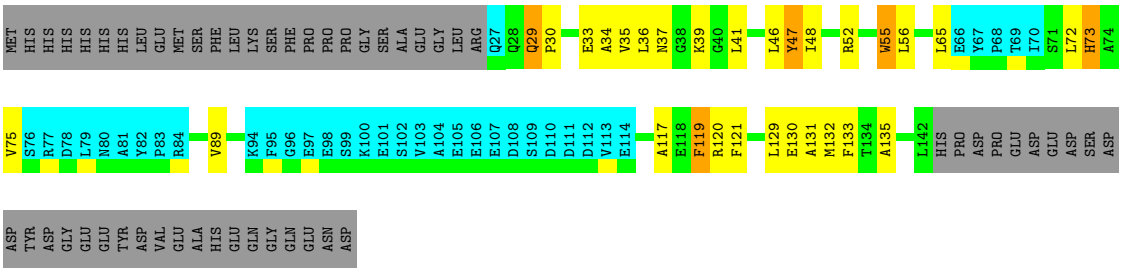
V75 S76 R77 D78 L79 N80 A81 Y82 P83 R84 L87 Y88 V89 M90 V91 K94 F95 G96 E97 E98 S99 K100 E101 S102 V103 A104 E105 E106 E107 D108 S109 D110 D111 D112 V113 E114 A117 E118 F119 R120 F121 V122 L129 T134 A135 E138 L142 HIS PRO ASP PRO GLU ASP

GLU ASP SER ASP ASP TYR ASP GLY GLU GLU TYR ASP VAL GLU ALA HIS GLU GLN GLY GLN GLU ASN ASP

4.2.8 Score per residue for model 8

• Molecule 1: Methylosome subunit pICln

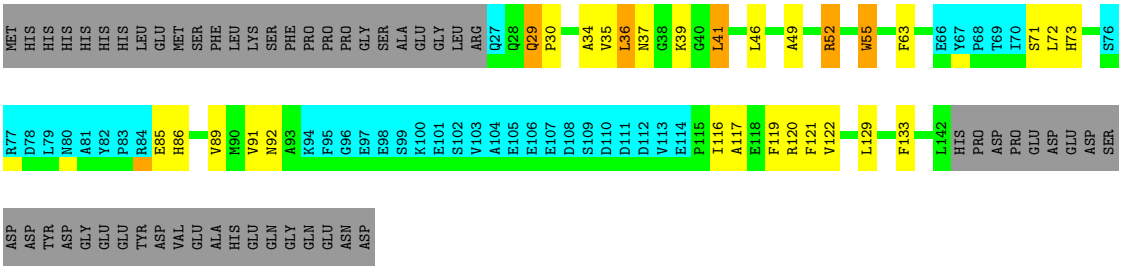
Chain A: 29% 15% • 21% 32%



4.2.9 Score per residue for model 9

- Molecule 1: Methylosome subunit pICln

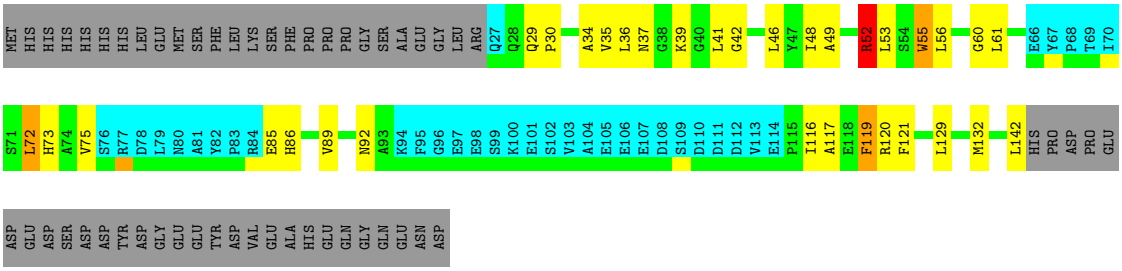
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: Methylosome subunit pICln

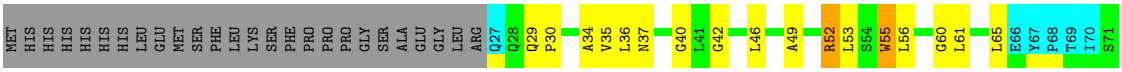
Chain A:

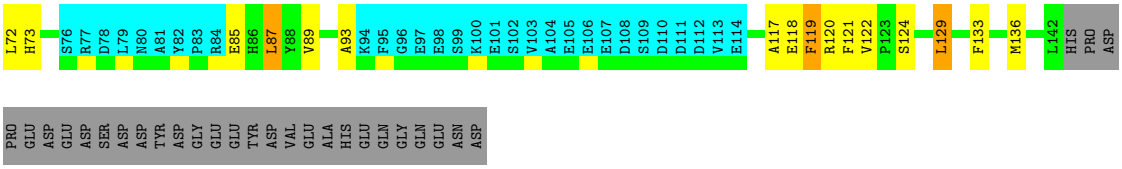


4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Methylosome subunit pICln

Chain A:

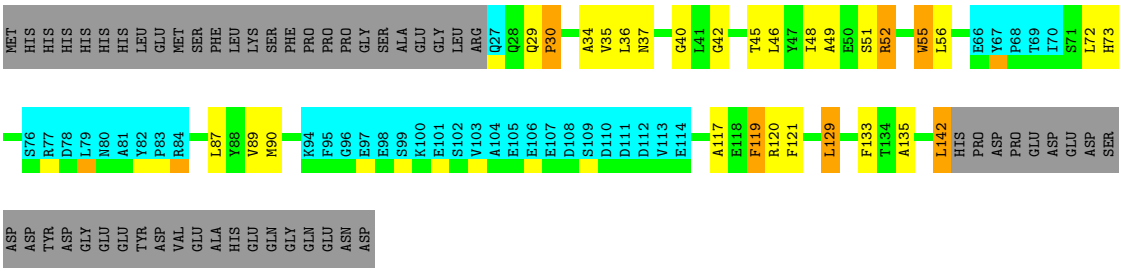




4.2.12 Score per residue for model 12

- Molecule 1: Methylosome subunit pICln

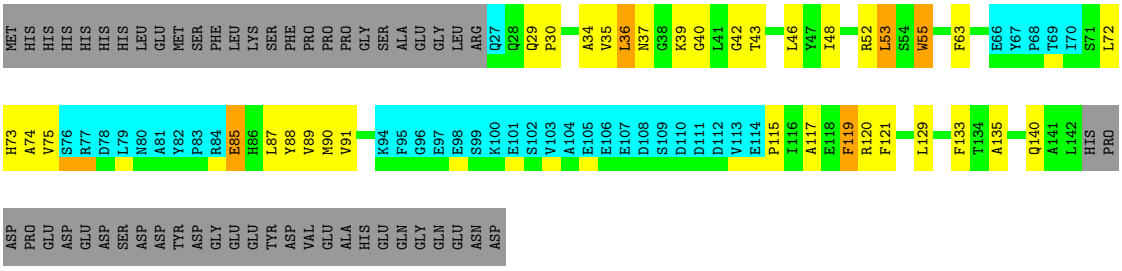
Chain A: 30% 13% • 21% 32%



4.2.13 Score per residue for model 13

- Molecule 1: Methylosome subunit pICln

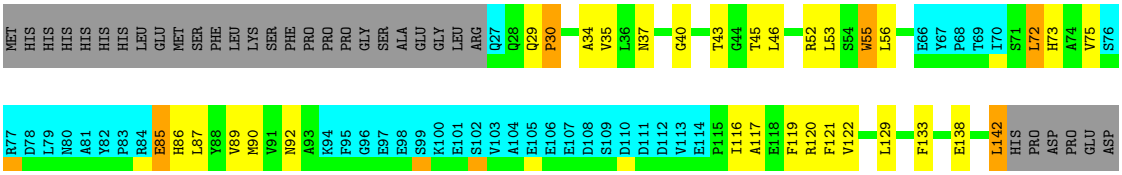
Chain A: 26% 18% • 21% 32%



4.2.14 Score per residue for model 14

- Molecule 1: Methylosome subunit pICln

Chain A: 28% 16% • 21% 32%



GLU ASP SER ASP ASP TYR ASP GLY GLU GLU GLU TYR ASP VAL GLU ALA HIS GLU GLN GLY GLN GLU ASN ASP

4.2.15 Score per residue for model 15

- Molecule 1: Methylosome subunit pICln

Chain A: 27% 16% • 21% 32%

MET HIS HIS HIS HIS HIS HIS LEU GLU MET SER PHE LEU LYS SER PHE PRO PRO PRO GLY SER ALA GLU GLY LEU ARG Q27 P30 E31 T32 E33 A34 V35 L36 N37 G38 K39 G40 T45 L46 A49 R52 L53 S54 W55 L56 F63 E66 Y67 P68 T69 I70 S71 L72

H73 A74 V75 S76 R77 D78 L79 N80 A81 Y82 P83 R84 E85 H86 L87 Y88 V89 M90 V91 K94 F95 G96 E97 E98 S99 K100 E101 S102 V103 A104 E105 E106 E107 D108 S109 D110 D111 D112 V113 E114 F119 R120 F121 V122 P123 L129 F133 L142 HIS PRO ASP PRO GLU ASP GLU

ASP SER ASP ASP TYR ASP GLY GLU GLU TYR ASP VAL GLU ALA HIS GLU GLN GLY GLN GLU ASN ASP

5 Refinement protocol and experimental data overview (i)

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

Of the 120 calculated structures, 15 were deposited, based on the following criterion: *structures with the least restraint violations and structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR-NIH	refinement	2.11

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.07±0.00	0±0/615 (0.0± 0.0%)	1.21±0.02	0±0/832 (0.0± 0.0%)
All	All	1.07	0/9225 (0.0%)	1.21	2/12480 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.0±0.0
All	All	0	30

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	119	PHE	N-CA-CB	-5.21	101.21	110.60	1	1
1	A	88	TYR	CB-CG-CD1	-5.04	117.98	121.00	3	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	52	ARG	Sidechain	15
1	A	120	ARG	Sidechain	15

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	603	591	591	29±5
All	All	9045	8865	8865	440

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:N	1:A:122:VAL:HG12	0.84	1.87	14	3
1:A:35:VAL:HG13	1:A:40:GLY:CA	0.78	2.08	3	6
1:A:89:VAL:HG22	1:A:119:PHE:CD1	0.76	2.15	9	14
1:A:30:PRO:O	1:A:45:THR:HG22	0.74	1.82	12	5
1:A:34:ALA:HB2	1:A:55:TRP:CZ2	0.72	2.19	11	15
1:A:85:GLU:CG	1:A:129:LEU:HD22	0.72	2.15	2	2
1:A:34:ALA:HB1	1:A:121:PHE:CZ	0.71	2.21	11	9
1:A:89:VAL:HG13	1:A:119:PHE:CD1	0.70	2.21	6	1
1:A:93:ALA:HB3	1:A:115:PRO:O	0.68	1.88	4	1
1:A:73:HIS:CB	1:A:89:VAL:HG12	0.67	2.18	11	10
1:A:49:ALA:HB3	1:A:52:ARG:O	0.67	1.90	11	9
1:A:72:LEU:O	1:A:72:LEU:HD13	0.65	1.91	14	1
1:A:35:VAL:HG13	1:A:39:LYS:O	0.65	1.90	5	4
1:A:75:VAL:CG2	1:A:129:LEU:HD11	0.65	2.22	5	1
1:A:92:ASN:CG	1:A:116:ILE:HD12	0.64	2.11	10	1
1:A:34:ALA:HB3	1:A:42:GLY:HA3	0.64	1.68	2	9
1:A:34:ALA:HB2	1:A:55:TRP:CH2	0.64	2.27	8	7
1:A:35:VAL:HG13	1:A:40:GLY:HA2	0.64	1.67	6	11
1:A:92:ASN:OD1	1:A:116:ILE:HG23	0.63	1.93	10	3
1:A:37:ASN:CB	1:A:117:ALA:HB1	0.63	2.24	13	4
1:A:48:ILE:HG21	1:A:135:ALA:HB1	0.63	1.69	7	1
1:A:29:GLN:O	1:A:45:THR:HG23	0.62	1.94	4	2
1:A:60:GLY:C	1:A:61:LEU:HD12	0.62	2.14	11	2
1:A:92:ASN:OD1	1:A:116:ILE:HD12	0.62	1.93	10	1
1:A:37:ASN:HB3	1:A:117:ALA:HB1	0.62	1.70	13	2
1:A:86:HIS:HA	1:A:122:VAL:HG13	0.62	1.71	3	3
1:A:29:GLN:OE1	1:A:131:ALA:HB3	0.61	1.94	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:SER:HB2	1:A:91:VAL:HG23	0.61	1.72	9	1
1:A:34:ALA:HB1	1:A:121:PHE:CE1	0.60	2.31	15	6
1:A:48:ILE:HD11	1:A:132:MET:CE	0.60	2.26	10	1
1:A:74:ALA:HB3	1:A:88:TYR:O	0.60	1.96	15	1
1:A:71:SER:HB3	1:A:91:VAL:HG22	0.60	1.74	5	1
1:A:72:LEU:HD23	1:A:72:LEU:O	0.59	1.97	11	11
1:A:85:GLU:HB3	1:A:129:LEU:HD13	0.58	1.73	6	4
1:A:71:SER:HB3	1:A:91:VAL:HG12	0.58	1.74	2	1
1:A:49:ALA:HB3	1:A:52:ARG:HG3	0.58	1.74	6	1
1:A:37:ASN:HB2	1:A:117:ALA:HB1	0.58	1.75	2	1
1:A:48:ILE:HD11	1:A:132:MET:SD	0.57	2.39	5	2
1:A:85:GLU:HB2	1:A:129:LEU:HD22	0.57	1.77	14	3
1:A:75:VAL:HG23	1:A:86:HIS:O	0.56	2.00	5	1
1:A:85:GLU:CB	1:A:129:LEU:HD22	0.56	2.30	3	6
1:A:89:VAL:HG13	1:A:119:PHE:CE1	0.56	2.36	6	1
1:A:72:LEU:HD22	1:A:90:MET:SD	0.56	2.40	12	3
1:A:48:ILE:HD12	1:A:48:ILE:N	0.55	2.16	12	2
1:A:119:PHE:CZ	1:A:121:PHE:CD1	0.55	2.94	3	15
1:A:73:HIS:NE2	1:A:87:LEU:HD11	0.55	2.16	15	1
1:A:65:LEU:HD12	1:A:65:LEU:N	0.55	2.16	1	2
1:A:35:VAL:HG13	1:A:40:GLY:HA3	0.55	1.79	3	3
1:A:36:LEU:HD13	1:A:37:ASN:HB2	0.55	1.79	4	1
1:A:72:LEU:HD12	1:A:90:MET:CE	0.54	2.33	14	1
1:A:129:LEU:HD11	1:A:133:PHE:CZ	0.54	2.37	1	3
1:A:119:PHE:CE1	1:A:121:PHE:CD1	0.54	2.96	9	15
1:A:71:SER:CB	1:A:91:VAL:HG12	0.53	2.34	2	1
1:A:48:ILE:HD13	1:A:135:ALA:CB	0.53	2.33	8	4
1:A:129:LEU:HD21	1:A:133:PHE:CZ	0.53	2.38	9	1
1:A:48:ILE:HD11	1:A:132:MET:HE3	0.52	1.81	10	1
1:A:119:PHE:CZ	1:A:121:PHE:CE1	0.52	2.97	6	6
1:A:142:LEU:HD13	1:A:142:LEU:O	0.52	2.05	15	2
1:A:56:LEU:C	1:A:56:LEU:HD13	0.52	2.25	2	11
1:A:120:ARG:HG2	1:A:122:VAL:HG23	0.51	1.82	2	3
1:A:85:GLU:HB2	1:A:129:LEU:HD13	0.51	1.81	3	2
1:A:37:ASN:CG	1:A:117:ALA:HB1	0.51	2.26	8	6
1:A:43:THR:HG23	1:A:43:THR:O	0.51	2.06	14	3
1:A:73:HIS:HA	1:A:89:VAL:HG12	0.51	1.82	7	4
1:A:89:VAL:HG22	1:A:119:PHE:HD1	0.51	1.61	9	2
1:A:87:LEU:H	1:A:122:VAL:HG12	0.50	1.65	7	2
1:A:85:GLU:HB3	1:A:129:LEU:HD22	0.50	1.83	9	1
1:A:119:PHE:CE2	1:A:121:PHE:CE1	0.50	2.99	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HB2	1:A:41:LEU:HD13	0.50	1.83	9	1
1:A:129:LEU:HD12	1:A:133:PHE:CZ	0.50	2.42	11	1
1:A:75:VAL:O	1:A:75:VAL:HG13	0.49	2.07	7	2
1:A:87:LEU:C	1:A:87:LEU:HD23	0.49	2.28	14	2
1:A:30:PRO:CA	1:A:45:THR:HG22	0.49	2.37	3	1
1:A:85:GLU:OE1	1:A:129:LEU:HD22	0.49	2.08	6	1
1:A:46:LEU:C	1:A:46:LEU:HD23	0.49	2.28	4	15
1:A:92:ASN:HA	1:A:116:ILE:HG23	0.49	1.85	9	3
1:A:72:LEU:HD23	1:A:72:LEU:C	0.49	2.28	8	7
1:A:72:LEU:HD22	1:A:90:MET:HE2	0.48	1.83	2	1
1:A:72:LEU:C	1:A:72:LEU:HD23	0.48	2.28	12	5
1:A:87:LEU:HD23	1:A:87:LEU:O	0.48	2.08	5	3
1:A:46:LEU:CD2	1:A:48:ILE:HD11	0.48	2.39	2	1
1:A:36:LEU:HD23	1:A:37:ASN:CG	0.48	2.29	3	1
1:A:87:LEU:CD2	1:A:129:LEU:HD12	0.48	2.38	7	1
1:A:46:LEU:HD21	1:A:53:LEU:HD21	0.48	1.85	13	2
1:A:75:VAL:CG1	1:A:87:LEU:HD12	0.48	2.38	14	1
1:A:87:LEU:HD23	1:A:88:TYR:N	0.48	2.24	15	1
1:A:89:VAL:CG2	1:A:119:PHE:CD1	0.47	2.98	2	11
1:A:87:LEU:HD23	1:A:87:LEU:C	0.47	2.30	5	1
1:A:36:LEU:HD13	1:A:36:LEU:C	0.47	2.30	4	1
1:A:85:GLU:HG2	1:A:129:LEU:HD22	0.47	1.86	10	2
1:A:73:HIS:HB2	1:A:89:VAL:HG12	0.47	1.86	8	3
1:A:37:ASN:OD1	1:A:117:ALA:HB1	0.47	2.10	7	2
1:A:36:LEU:CB	1:A:41:LEU:HD13	0.47	2.40	9	1
1:A:85:GLU:HG3	1:A:129:LEU:HD22	0.47	1.87	2	1
1:A:85:GLU:HA	1:A:129:LEU:HD22	0.47	1.86	13	1
1:A:71:SER:CB	1:A:91:VAL:HG22	0.47	2.39	5	1
1:A:72:LEU:C	1:A:72:LEU:HD12	0.46	2.31	10	1
1:A:48:ILE:HD13	1:A:135:ALA:HB1	0.46	1.87	8	1
1:A:138:GLU:O	1:A:142:LEU:HD12	0.46	2.10	14	1
1:A:41:LEU:HD12	1:A:41:LEU:O	0.46	2.11	2	1
1:A:47:TYR:CE2	1:A:54:SER:CB	0.46	2.99	4	1
1:A:36:LEU:HD23	1:A:37:ASN:ND2	0.46	2.26	13	1
1:A:46:LEU:HD12	1:A:55:TRP:HE1	0.46	1.70	3	2
1:A:88:TYR:CD1	1:A:120:ARG:CB	0.46	2.99	6	1
1:A:63:PHE:N	1:A:63:PHE:CD1	0.46	2.83	2	6
1:A:134:THR:HG22	1:A:138:GLU:OE2	0.46	2.11	5	2
1:A:34:ALA:CB	1:A:55:TRP:CH2	0.45	3.00	6	3
1:A:123:PRO:CD	1:A:129:LEU:HD13	0.45	2.41	15	1
1:A:47:TYR:CD1	1:A:47:TYR:N	0.45	2.84	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LEU:CD1	1:A:133:PHE:CE1	0.45	3.00	4	3
1:A:75:VAL:CG1	1:A:133:PHE:CE1	0.45	3.00	3	1
1:A:36:LEU:HD23	1:A:37:ASN:OD1	0.45	2.11	3	1
1:A:29:GLN:OE1	1:A:46:LEU:HD22	0.45	2.12	9	1
1:A:75:VAL:CG2	1:A:133:PHE:CE1	0.45	3.00	2	1
1:A:75:VAL:HG13	1:A:133:PHE:CZ	0.45	2.46	8	1
1:A:34:ALA:CB	1:A:55:TRP:CZ2	0.44	3.00	4	5
1:A:129:LEU:CD1	1:A:133:PHE:CZ	0.44	3.00	12	4
1:A:34:ALA:HB2	1:A:55:TRP:CE2	0.44	2.47	4	1
1:A:45:THR:HG22	1:A:56:LEU:HB3	0.44	1.89	7	1
1:A:32:THR:HG23	1:A:123:PRO:CA	0.44	2.43	1	1
1:A:88:TYR:CE1	1:A:120:ARG:CB	0.44	3.01	6	1
1:A:75:VAL:HG11	1:A:133:PHE:CE1	0.44	2.48	14	2
1:A:138:GLU:O	1:A:142:LEU:HD23	0.44	2.13	5	1
1:A:119:PHE:CE1	1:A:121:PHE:CG	0.44	3.06	4	1
1:A:86:HIS:CD2	1:A:122:VAL:HG11	0.43	2.48	3	1
1:A:72:LEU:HD12	1:A:90:MET:HE3	0.43	1.89	14	1
1:A:72:LEU:HD22	1:A:90:MET:CE	0.43	2.43	2	1
1:A:92:ASN:CA	1:A:116:ILE:HG23	0.43	2.44	9	1
1:A:34:ALA:CB	1:A:121:PHE:CZ	0.43	3.00	1	1
1:A:35:VAL:HG11	1:A:120:ARG:HE	0.43	1.73	6	1
1:A:129:LEU:CD2	1:A:133:PHE:CZ	0.43	3.02	9	1
1:A:72:LEU:HD22	1:A:90:MET:HB2	0.43	1.89	15	1
1:A:49:ALA:HB3	1:A:52:ARG:C	0.42	2.35	11	1
1:A:89:VAL:O	1:A:119:PHE:O	0.42	2.37	6	1
1:A:87:LEU:HD22	1:A:129:LEU:HD12	0.42	1.91	7	1
1:A:73:HIS:CA	1:A:89:VAL:HG12	0.42	2.44	13	2
1:A:86:HIS:CD2	1:A:86:HIS:N	0.42	2.88	14	1
1:A:46:LEU:HD22	1:A:48:ILE:HD11	0.42	1.91	2	1
1:A:73:HIS:NE2	1:A:87:LEU:HD12	0.42	2.29	7	1
1:A:87:LEU:HD22	1:A:89:VAL:HG13	0.42	1.92	15	1
1:A:123:PRO:HD2	1:A:129:LEU:HD13	0.42	1.92	15	1
1:A:88:TYR:CD1	1:A:120:ARG:HB3	0.42	2.50	6	1
1:A:30:PRO:HA	1:A:45:THR:HG22	0.42	1.91	3	1
1:A:35:VAL:HA	1:A:40:GLY:HA2	0.41	1.92	1	2
1:A:87:LEU:HD21	1:A:136:MET:CE	0.41	2.46	1	1
1:A:75:VAL:HG12	1:A:87:LEU:HG	0.41	1.91	4	1
1:A:75:VAL:HG12	1:A:87:LEU:HD12	0.41	1.92	14	1
1:A:71:SER:HB2	1:A:91:VAL:HG22	0.41	1.92	15	1
1:A:87:LEU:CD2	1:A:89:VAL:HG13	0.41	2.46	15	1
1:A:32:THR:HG23	1:A:123:PRO:HA	0.41	1.92	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:HIS:CE1	1:A:140:GLN:NE2	0.41	2.89	13	1
1:A:74:ALA:HB3	1:A:88:TYR:HB3	0.41	1.92	13	1
1:A:63:PHE:CD1	1:A:63:PHE:N	0.41	2.89	15	1
1:A:29:GLN:HG3	1:A:128:ALA:HB1	0.41	1.93	2	1
1:A:35:VAL:HG11	1:A:120:ARG:NE	0.41	2.31	6	1
1:A:55:TRP:CZ3	1:A:56:LEU:O	0.41	2.74	15	3
1:A:32:THR:HG23	1:A:123:PRO:HB3	0.41	1.92	15	1
1:A:47:TYR:CE2	1:A:54:SER:HB2	0.41	2.50	4	1
1:A:29:GLN:NE2	1:A:46:LEU:HD22	0.41	2.31	14	1
1:A:75:VAL:O	1:A:86:HIS:CE1	0.40	2.75	10	2
1:A:37:ASN:ND2	1:A:117:ALA:CB	0.40	2.85	9	2
1:A:86:HIS:ND1	1:A:122:VAL:CG1	0.40	2.84	9	1
1:A:61:LEU:CD1	1:A:61:LEU:N	0.40	2.84	11	1
1:A:37:ASN:HA	1:A:118:GLU:N	0.40	2.31	2	1
1:A:73:HIS:O	1:A:73:HIS:CD2	0.40	2.75	5	1
1:A:35:VAL:HG21	1:A:120:ARG:NH2	0.40	2.31	6	1
1:A:61:LEU:HD12	1:A:61:LEU:N	0.40	2.30	11	1
1:A:73:HIS:NE2	1:A:87:LEU:CD1	0.40	2.85	7	1
1:A:73:HIS:CD2	1:A:73:HIS:O	0.40	2.75	11	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	79/171 (46%)	73±1 (92±2%)	5±1 (6±2%)	1±1 (2±1%)	12	54
All	All	1185/2565 (46%)	1093 (92%)	71 (6%)	21 (2%)	12	54

All 5 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	30	PRO	14
1	A	42	GLY	2
1	A	75	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	85	GLU	2
1	A	115	PRO	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	64/146 (44%)	57±2 (89±4%)	7±2 (11±4%)	9 53
All	All	960/2190 (44%)	853 (89%)	107 (11%)	9 53

All 28 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	55	TRP	15
1	A	36	LEU	13
1	A	119	PHE	10
1	A	53	LEU	8
1	A	29	GLN	8
1	A	142	LEU	7
1	A	71	SER	4
1	A	41	LEU	4
1	A	87	LEU	4
1	A	63	PHE	3
1	A	33	GLU	3
1	A	85	GLU	3
1	A	129	LEU	3
1	A	47	TYR	2
1	A	37	ASN	2
1	A	52	ARG	2
1	A	124	SER	2
1	A	136	MET	2
1	A	72	LEU	2
1	A	39	LYS	2
1	A	31	GLU	1
1	A	57	ASP	1
1	A	125	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	65	LEU	1
1	A	73	HIS	1
1	A	130	GLU	1
1	A	118	GLU	1
1	A	51	SER	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)

No chemical shift data were provided