



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:07 AM BST

PDB ID : 2MZE
Title : NMR Solution Structure of the PRO Form of Human Matrilysin (proMMP-7)
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Deposited on : 2015-02-11

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

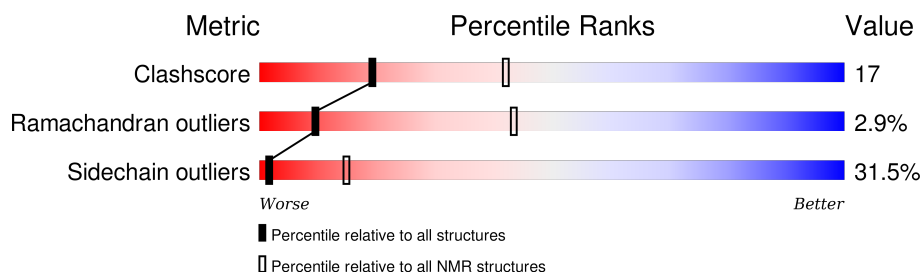
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	250	<div> <div></div> <div>45%</div> <div>29%</div> <div>6%</div> <div>20%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:12-A:23, A:35-A:72, A:82-A:216, A:224-A:239 (201)	0.37	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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3883 atoms, of which 1913 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrilysin.

Mol	Chain	Residues	Atoms						Trace
1	A	250	Total	C	H	N	O	S	0
			3879	1251	1913	341	365	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	GLU	ENGINEERED MUTATION	UNP P09237

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

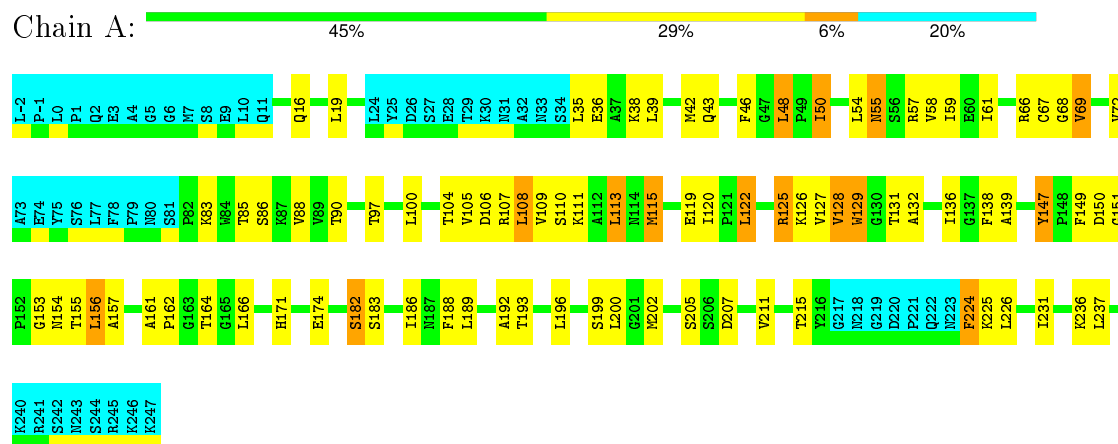
Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

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: Matrilysin

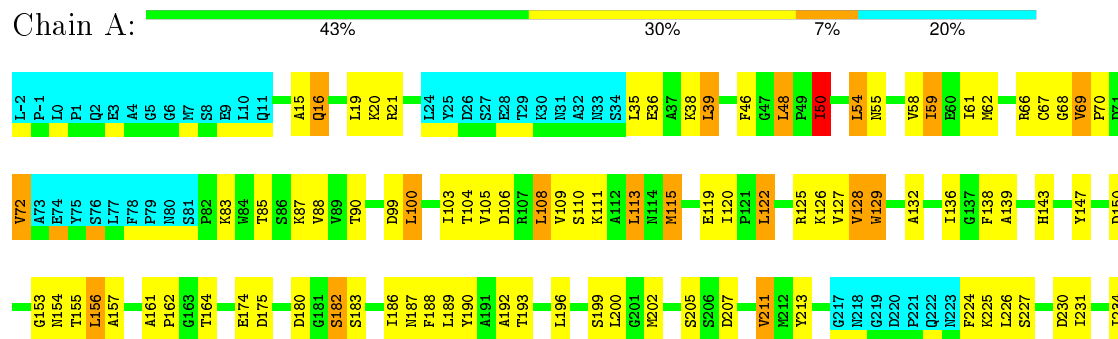


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

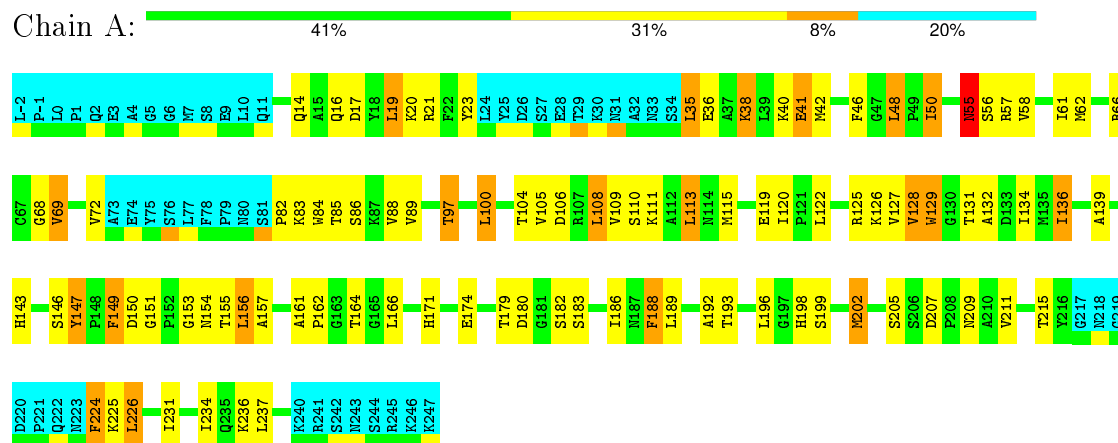
- Molecule 1: Matrilysin





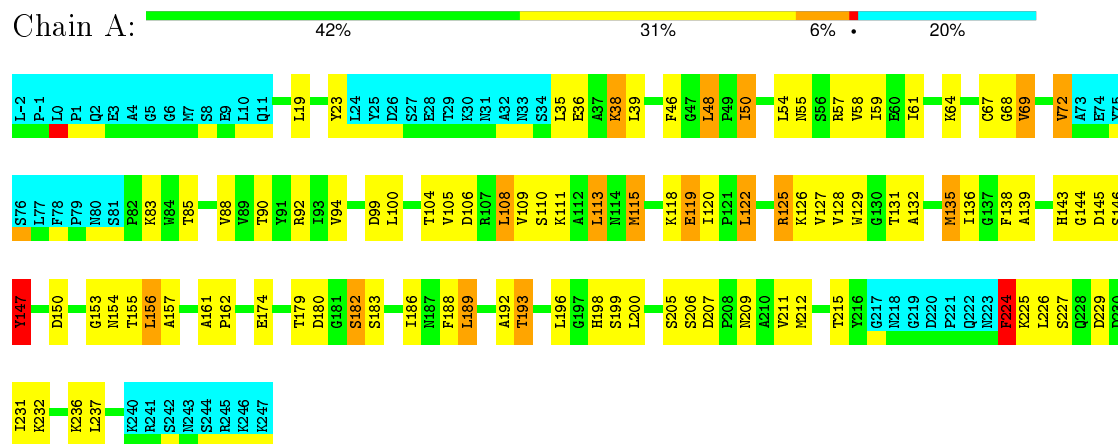
4.2.2 Score per residue for model 2

- Molecule 1: Matrilysin



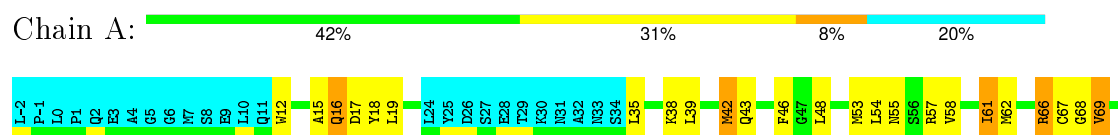
4.2.3 Score per residue for model 3

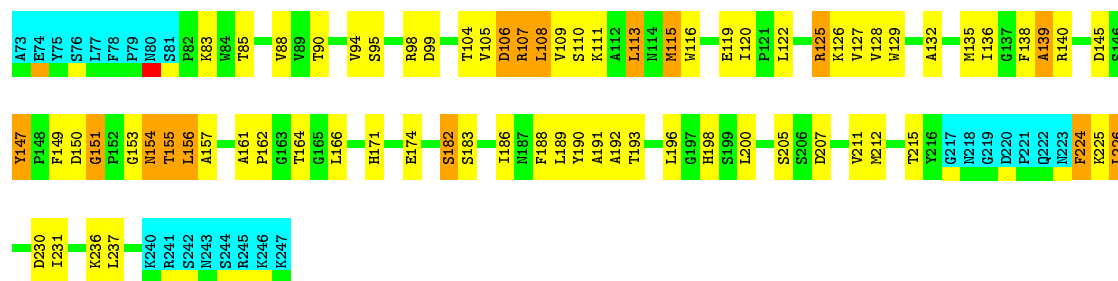
- Molecule 1: Matrilysin



4.2.4 Score per residue for model 4

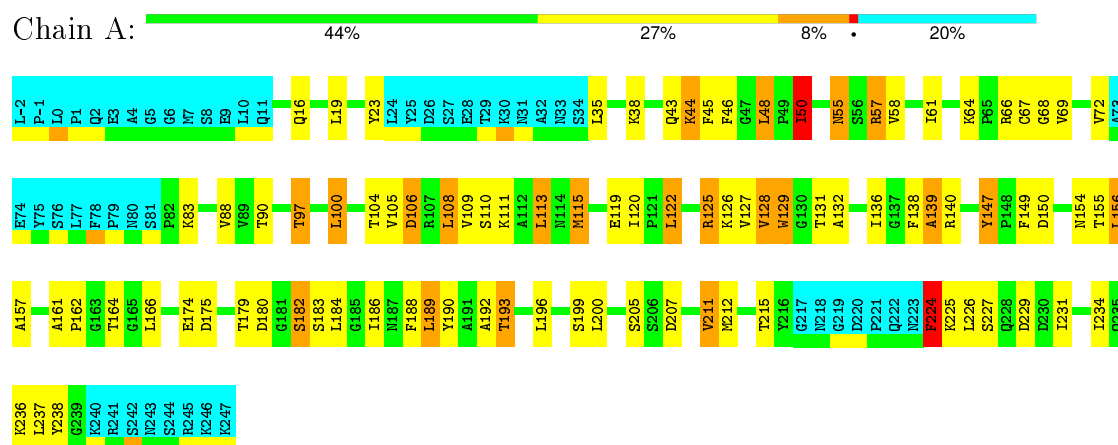
- Molecule 1: Matrilysin





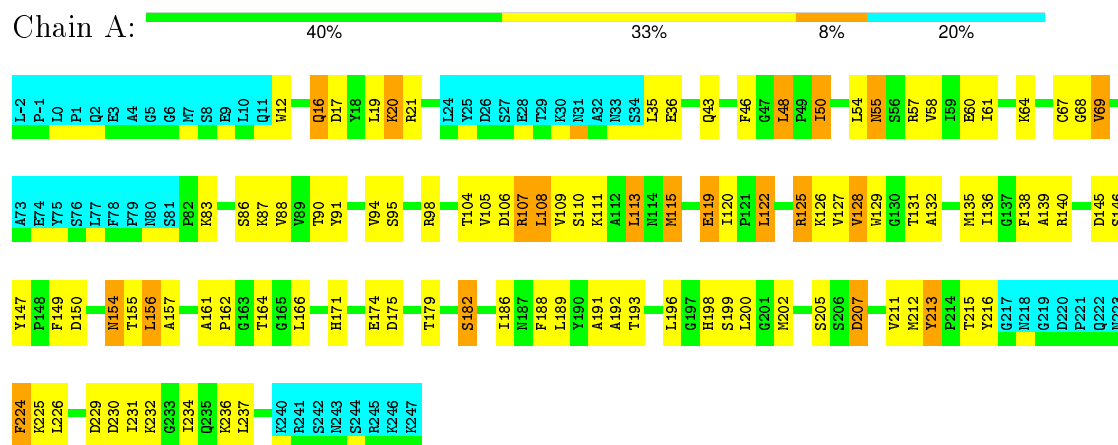
4.2.5 Score per residue for model 5

- Molecule 1: Matrilysin



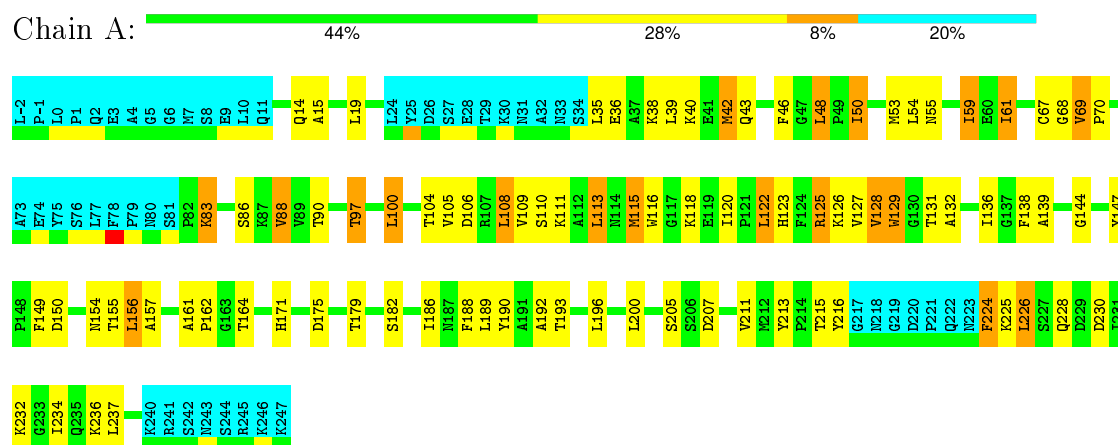
4.2.6 Score per residue for model 6

- Molecule 1: Matrilysin



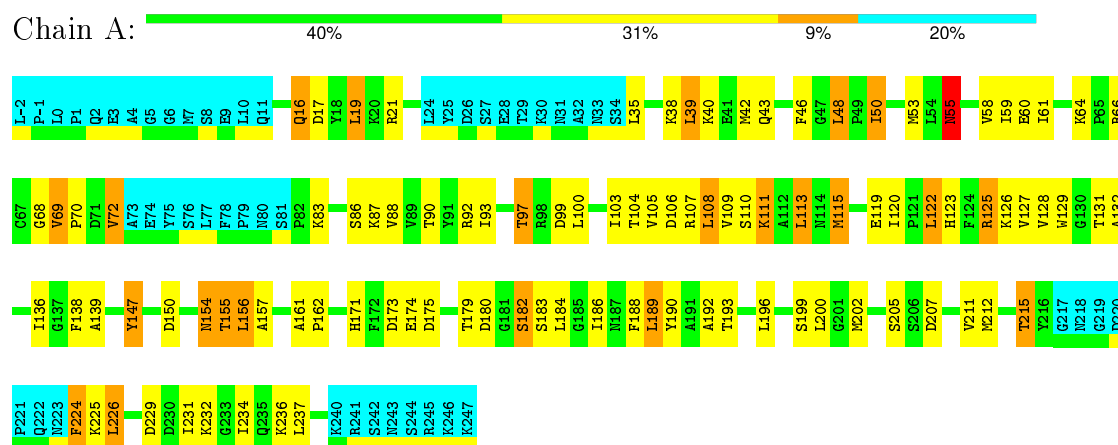
4.2.7 Score per residue for model 7

• Molecule 1: Matrilysin



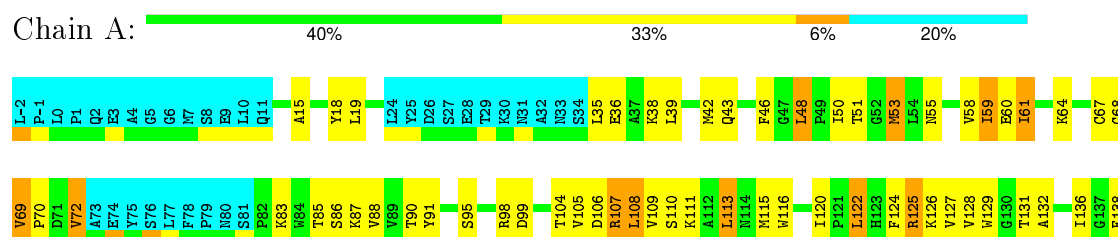
4.2.8 Score per residue for model 8

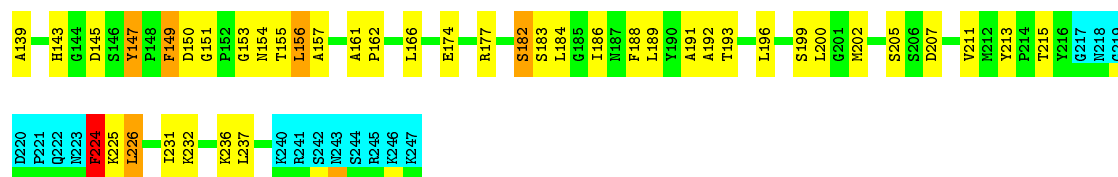
• Molecule 1: Matrilysin



4.2.9 Score per residue for model 9

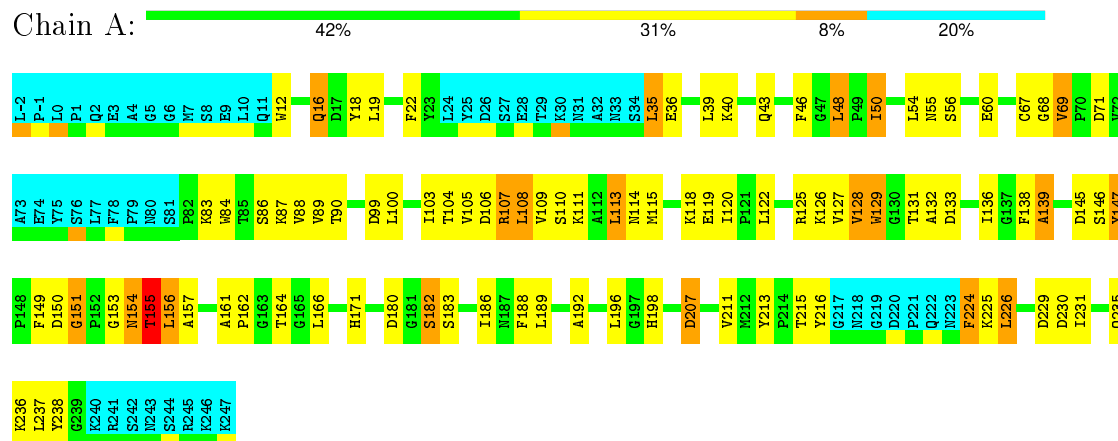
• Molecule 1: Matrilysin





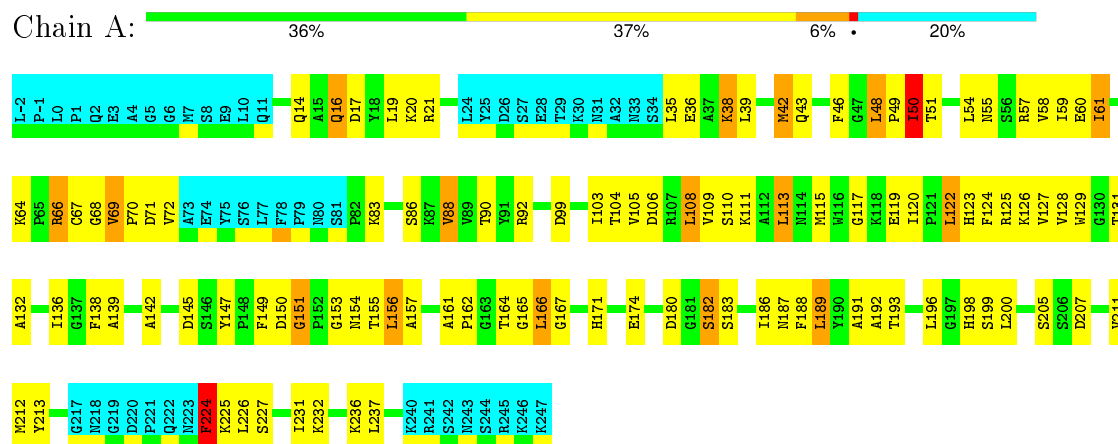
4.2.10 Score per residue for model 10

- Molecule 1: Matrilysin



4.2.11 Score per residue for model 11

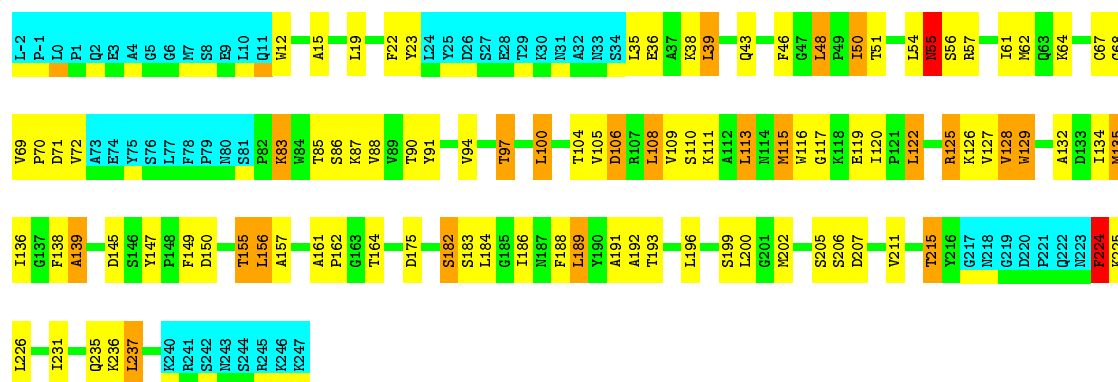
- Molecule 1: Matrilysin



4.2.12 Score per residue for model 12

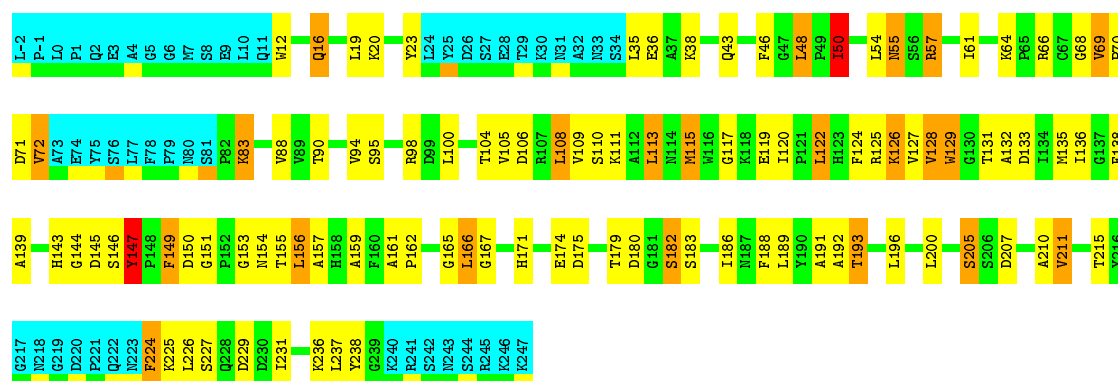
- Molecule 1: Matrilysin





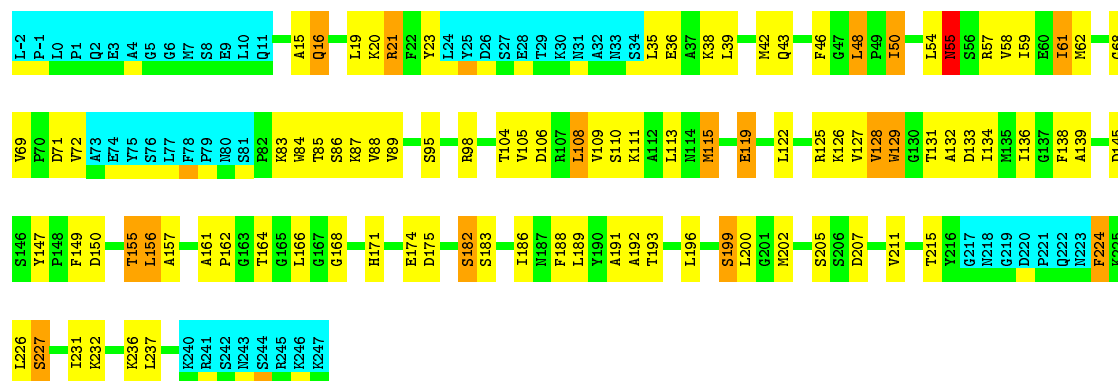
4.2.13 Score per residue for model 13

- Molecule 1: Matrilysin



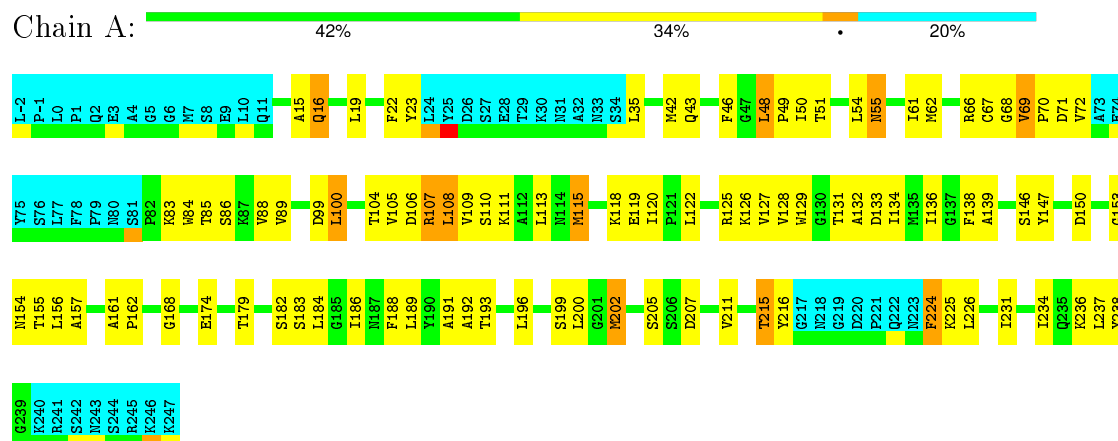
4.2.14 Score per residue for model 14

- Molecule 1: Matrilysin



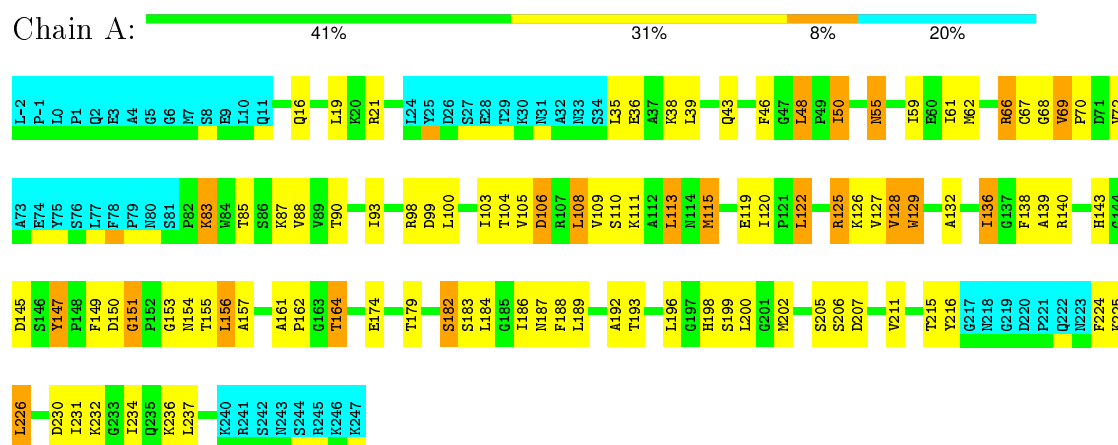
4.2.15 Score per residue for model 15

• Molecule 1: Matrilysin



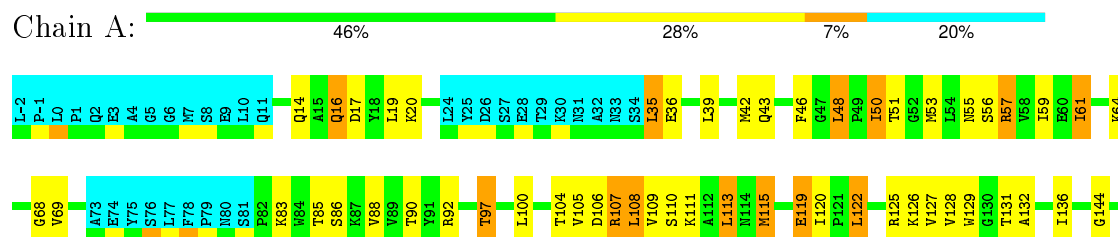
4.2.16 Score per residue for model 16

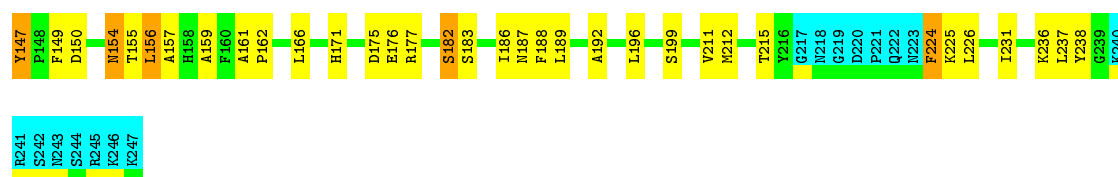
• Molecule 1: Matrilysin



4.2.17 Score per residue for model 17

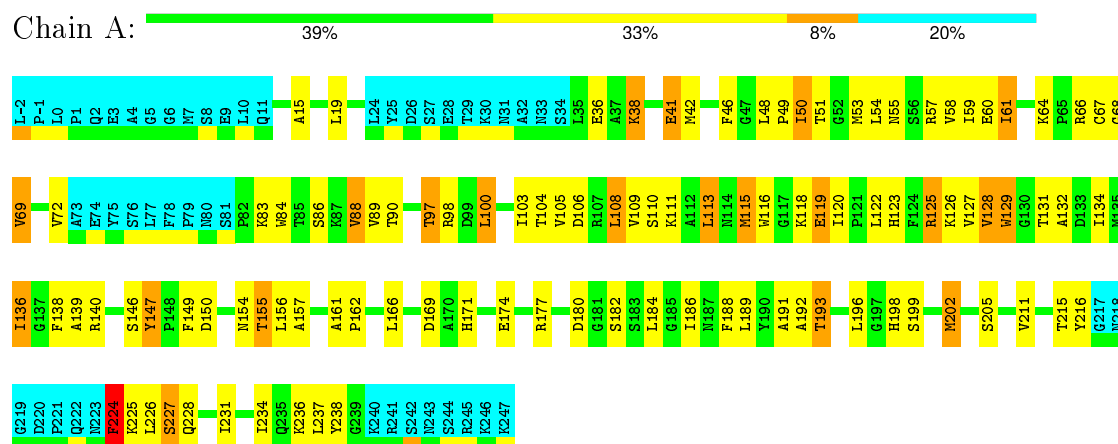
• Molecule 1: Matrilysin





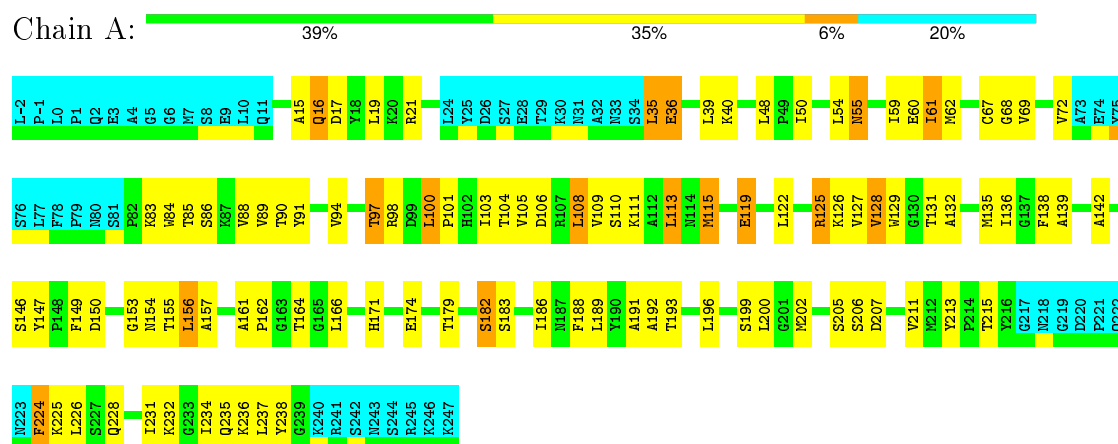
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Matrilysin



4.2.19 Score per residue for model 19

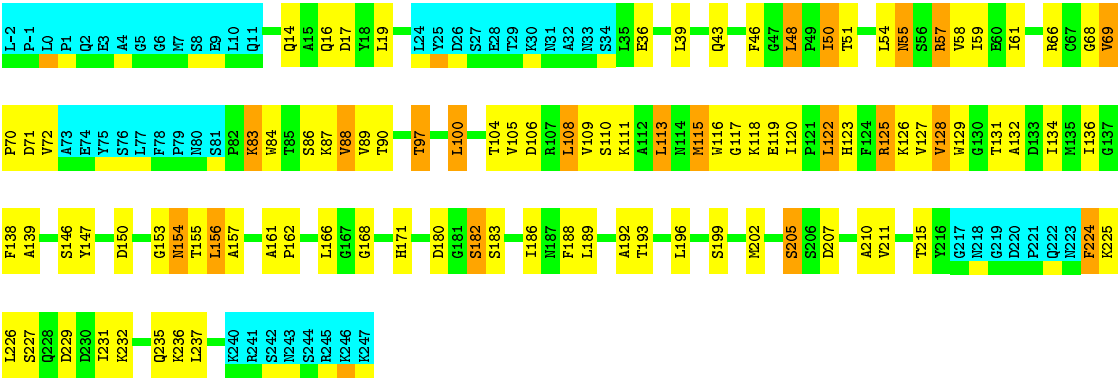
- Molecule 1: Matrilysin



4.2.20 Score per residue for model 20

- Molecule 1: Matrilysin





5 Refinement protocol and experimental data overview

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

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
TALOS	geometry optimization	
CYANA	structure solution	2.1
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)	2mze_cs.str
Number of chemical shift lists	1
Total number of shifts	2659
Number of shifts mapped to atoms	2659
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	1590	1555	1556	52±6
All	All	31880	31100	31120	1046

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ILE:HD12	1:A:122:LEU:HD12	0.97	1.34	3	18
1:A:156:LEU:HD21	1:A:186:ILE:HG21	0.96	1.38	5	20
1:A:127:VAL:HG11	1:A:132:ALA:HB2	0.94	1.37	7	20
1:A:113:LEU:HD13	1:A:196:LEU:HD12	0.91	1.39	14	7
1:A:39:LEU:HD11	1:A:54:LEU:HD22	0.81	1.53	3	3
1:A:83:LYS:HD2	1:A:237:LEU:HD23	0.78	1.56	12	2
1:A:43:GLN:HA	1:A:48:LEU:HD12	0.77	1.54	4	2
1:A:46:PHE:CZ	1:A:61:ILE:HD13	0.75	2.17	20	6
1:A:166:LEU:C	1:A:166:LEU:HD22	0.73	2.04	13	2
1:A:156:LEU:HD21	1:A:186:ILE:CG2	0.72	2.14	6	20
1:A:113:LEU:CD1	1:A:196:LEU:HD12	0.70	2.16	11	20
1:A:105:VAL:O	1:A:109:VAL:HG13	0.69	1.87	10	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:VAL:HG13	1:A:188:PHE:CZ	0.69	2.23	15	19
1:A:104:THR:O	1:A:108:LEU:HD22	0.68	1.89	17	20
1:A:113:LEU:HD12	1:A:196:LEU:HD12	0.68	1.65	17	18
1:A:115:MET:HB3	1:A:226:LEU:HD23	0.68	1.65	16	5
1:A:68:GLY:CA	1:A:155:THR:HG23	0.67	2.19	8	1
1:A:115:MET:O	1:A:226:LEU:HD11	0.67	1.88	5	11
1:A:43:GLN:OE1	1:A:48:LEU:HD11	0.67	1.90	16	5
1:A:84:TRP:CE3	1:A:89:VAL:HG21	0.66	2.26	18	7
1:A:83:LYS:HD2	1:A:237:LEU:HD22	0.65	1.66	4	11
1:A:192:ALA:O	1:A:196:LEU:HD23	0.65	1.91	10	20
1:A:39:LEU:HD13	1:A:54:LEU:HD23	0.65	1.68	11	2
1:A:83:LYS:CE	1:A:237:LEU:HD13	0.65	2.21	15	10
1:A:19:LEU:HD13	1:A:19:LEU:O	0.64	1.92	20	6
1:A:226:LEU:HB3	1:A:231:ILE:HD11	0.64	1.70	9	12
1:A:53:MET:O	1:A:58:VAL:HG21	0.63	1.94	4	2
1:A:83:LYS:HE3	1:A:237:LEU:HD13	0.63	1.68	4	1
1:A:83:LYS:CD	1:A:237:LEU:HD22	0.63	2.24	16	5
1:A:166:LEU:HD22	1:A:167:GLY:N	0.63	2.09	11	2
1:A:39:LEU:CD1	1:A:54:LEU:HD23	0.63	2.23	14	2
1:A:127:VAL:HG11	1:A:132:ALA:CB	0.63	2.22	9	14
1:A:119:GLU:HG2	1:A:226:LEU:HD13	0.63	1.70	14	7
1:A:68:GLY:HA2	1:A:155:THR:HG23	0.63	1.69	8	9
1:A:193:THR:HG21	1:A:211:VAL:HG21	0.63	1.69	5	3
1:A:83:LYS:CG	1:A:237:LEU:HD22	0.62	2.24	7	3
1:A:42:MET:CE	1:A:61:ILE:HD11	0.62	2.24	4	6
1:A:94:VAL:HG22	1:A:135:MET:SD	0.61	2.35	19	6
1:A:61:ILE:HG21	1:A:215:THR:HG22	0.61	1.72	19	2
1:A:46:PHE:CD2	1:A:61:ILE:HD12	0.61	2.30	4	2
1:A:120:ILE:CD1	1:A:122:LEU:HD12	0.61	2.26	16	13
1:A:54:LEU:CD1	1:A:59:ILE:HD13	0.61	2.25	20	1
1:A:119:GLU:HB3	1:A:231:ILE:HG23	0.61	1.72	2	7
1:A:46:PHE:CE2	1:A:61:ILE:HD13	0.61	2.30	6	2
1:A:43:GLN:CB	1:A:51:THR:HG22	0.60	2.26	20	3
1:A:69:VAL:HG12	1:A:70:PRO:HD2	0.60	1.73	7	8
1:A:16:GLN:NE2	1:A:35:LEU:HD12	0.60	2.11	17	6
1:A:43:GLN:CA	1:A:48:LEU:HD12	0.60	2.26	4	2
1:A:50:ILE:HD13	1:A:56:SER:OG	0.60	1.97	12	1
1:A:83:LYS:HD3	1:A:237:LEU:HD22	0.60	1.72	17	6
1:A:19:LEU:O	1:A:19:LEU:HD13	0.60	1.96	13	5
1:A:46:PHE:CG	1:A:61:ILE:HD12	0.60	2.32	4	1
1:A:127:VAL:CG1	1:A:132:ALA:HB2	0.60	2.27	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:ALA:HB1	1:A:162:PRO:HD2	0.59	1.74	14	20
1:A:134:ILE:HG23	1:A:168:GLY:O	0.59	1.97	20	3
1:A:119:GLU:HG3	1:A:226:LEU:HD13	0.59	1.74	10	2
1:A:237:LEU:HD23	1:A:237:LEU:O	0.59	1.98	19	4
1:A:69:VAL:HG21	1:A:198:HIS:CD2	0.59	2.32	4	8
1:A:84:TRP:CH2	1:A:89:VAL:HG11	0.59	2.33	20	4
1:A:49:PRO:O	1:A:51:THR:HG23	0.59	1.97	15	3
1:A:57:ARG:O	1:A:61:ILE:HG23	0.58	1.97	20	10
1:A:68:GLY:N	1:A:157:ALA:O	0.58	2.34	10	20
1:A:43:GLN:HG2	1:A:48:LEU:HD11	0.58	1.73	12	6
1:A:16:GLN:HB3	1:A:35:LEU:HD21	0.58	1.76	10	1
1:A:119:GLU:HB2	1:A:231:ILE:HG23	0.58	1.74	15	1
1:A:61:ILE:CG2	1:A:215:THR:HG22	0.58	2.29	19	1
1:A:90:THR:HG22	1:A:125:ARG:HB3	0.58	1.76	19	12
1:A:237:LEU:O	1:A:237:LEU:HD23	0.58	1.98	4	7
1:A:134:ILE:HD12	1:A:134:ILE:N	0.57	2.14	18	2
1:A:69:VAL:HG21	1:A:159:ALA:O	0.57	2.00	17	2
1:A:134:ILE:N	1:A:134:ILE:HD12	0.57	2.14	2	1
1:A:83:LYS:CD	1:A:237:LEU:HD13	0.57	2.29	11	10
1:A:46:PHE:CE2	1:A:61:ILE:HD12	0.57	2.35	1	5
1:A:166:LEU:HD13	1:A:166:LEU:O	0.57	2.00	14	1
1:A:106:ASP:O	1:A:109:VAL:HG22	0.57	2.00	16	20
1:A:39:LEU:CD1	1:A:54:LEU:HD22	0.56	2.28	3	2
1:A:43:GLN:CD	1:A:48:LEU:HD11	0.56	2.21	13	5
1:A:83:LYS:HD2	1:A:237:LEU:HD13	0.56	1.77	17	6
1:A:138:PHE:O	1:A:139:ALA:HB2	0.56	2.01	12	18
1:A:46:PHE:HB3	1:A:48:LEU:HD23	0.56	1.77	1	6
1:A:122:LEU:HD11	1:A:238:TYR:CZ	0.56	2.36	13	2
1:A:100:LEU:HD22	1:A:104:THR:HG21	0.56	1.77	3	5
1:A:166:LEU:HD23	1:A:166:LEU:O	0.56	2.00	10	2
1:A:16:GLN:CD	1:A:35:LEU:HD12	0.56	2.21	8	1
1:A:189:LEU:HD12	1:A:224:PHE:CD2	0.55	2.37	3	3
1:A:42:MET:HE1	1:A:61:ILE:HD11	0.55	1.79	11	1
1:A:19:LEU:HD12	1:A:38:LYS:HG2	0.55	1.78	3	1
1:A:43:GLN:HA	1:A:48:LEU:CD1	0.55	2.32	17	1
1:A:16:GLN:NE2	1:A:35:LEU:HD22	0.55	2.16	5	3
1:A:202:MET:SD	1:A:234:ILE:HD12	0.55	2.41	16	6
1:A:15:ALA:HB1	1:A:62:MET:CE	0.55	2.31	19	2
1:A:46:PHE:CZ	1:A:61:ILE:HD12	0.54	2.37	11	7
1:A:226:LEU:CB	1:A:231:ILE:HD11	0.54	2.33	18	3
1:A:226:LEU:HD22	1:A:231:ILE:HD11	0.54	1.77	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:CD1	1:A:109:VAL:HG11	0.54	2.32	8	1
1:A:97:THR:O	1:A:100:LEU:O	0.54	2.26	8	9
1:A:46:PHE:CE1	1:A:61:ILE:HD12	0.54	2.38	17	2
1:A:42:MET:HE3	1:A:61:ILE:HD11	0.54	1.79	4	3
1:A:105:VAL:HG13	1:A:188:PHE:CE2	0.54	2.37	11	9
1:A:166:LEU:O	1:A:166:LEU:HD23	0.54	2.01	5	3
1:A:116:TRP:O	1:A:119:GLU:HG3	0.54	2.03	12	1
1:A:39:LEU:HD21	1:A:54:LEU:HD22	0.54	1.80	4	1
1:A:42:MET:HE1	1:A:58:VAL:HG13	0.54	1.80	9	1
1:A:15:ALA:HB1	1:A:62:MET:HE3	0.53	1.81	14	5
1:A:186:ILE:HG22	1:A:191:ALA:HB2	0.53	1.81	12	10
1:A:100:LEU:HD21	1:A:179:THR:HA	0.53	1.79	13	6
1:A:50:ILE:HD11	1:A:57:ARG:HG2	0.53	1.80	13	1
1:A:166:LEU:C	1:A:166:LEU:CD2	0.53	2.76	11	2
1:A:226:LEU:HD23	1:A:230:ASP:OD2	0.53	2.04	10	1
1:A:50:ILE:HD12	1:A:58:VAL:HG23	0.53	1.81	5	10
1:A:19:LEU:HD21	1:A:42:MET:HG3	0.53	1.80	7	2
1:A:149:PHE:O	1:A:150:ASP:CG	0.53	2.47	13	7
1:A:119:GLU:OE1	1:A:120:ILE:HG23	0.53	2.04	12	1
1:A:100:LEU:HD21	1:A:180:ASP:H	0.52	1.62	8	1
1:A:19:LEU:HD13	1:A:38:LYS:HG2	0.52	1.79	18	1
1:A:15:ALA:CB	1:A:54:LEU:HD21	0.52	2.33	18	2
1:A:19:LEU:HD22	1:A:23:TYR:CE2	0.52	2.39	2	1
1:A:134:ILE:CD1	1:A:134:ILE:N	0.52	2.73	18	1
1:A:139:ALA:HB1	1:A:143:HIS:CB	0.52	2.34	3	6
1:A:39:LEU:HD21	1:A:54:LEU:CD2	0.52	2.34	4	1
1:A:54:LEU:HD13	1:A:59:ILE:HD13	0.52	1.82	20	1
1:A:128:VAL:HG23	1:A:129:TRP:NE1	0.52	2.20	5	10
1:A:142:ALA:HB2	1:A:149:PHE:CD2	0.52	2.40	11	2
1:A:39:LEU:HD21	1:A:54:LEU:HB2	0.51	1.82	12	2
1:A:116:TRP:CZ3	1:A:226:LEU:HD11	0.51	2.41	4	3
1:A:83:LYS:HE2	1:A:237:LEU:HD13	0.51	1.81	15	2
1:A:156:LEU:HD11	1:A:186:ILE:HG13	0.51	1.82	3	2
1:A:119:GLU:CG	1:A:226:LEU:HD13	0.51	2.36	2	3
1:A:16:GLN:NE2	1:A:35:LEU:HD13	0.50	2.21	6	1
1:A:35:LEU:O	1:A:39:LEU:HG	0.50	2.06	9	4
1:A:117:GLY:HA2	1:A:120:ILE:CG1	0.50	2.37	11	4
1:A:54:LEU:CD1	1:A:59:ILE:HD12	0.50	2.36	1	1
1:A:46:PHE:CB	1:A:48:LEU:HD23	0.50	2.37	12	14
1:A:84:TRP:CZ3	1:A:89:VAL:HG11	0.50	2.42	2	5
1:A:109:VAL:CG2	1:A:110:SER:N	0.49	2.74	6	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ILE:HD13	1:A:215:THR:HG22	0.49	1.83	9	1
1:A:134:ILE:HG22	1:A:136:ILE:CD1	0.49	2.37	18	2
1:A:61:ILE:HG21	1:A:215:THR:HG23	0.49	1.83	15	1
1:A:19:LEU:HD13	1:A:39:LEU:HD22	0.49	1.84	8	1
1:A:35:LEU:CD2	1:A:39:LEU:HD22	0.49	2.37	7	1
1:A:88:VAL:HG23	1:A:123:HIS:CD2	0.49	2.42	20	5
1:A:139:ALA:HB1	1:A:143:HIS:HB3	0.49	1.85	13	3
1:A:146:SER:O	1:A:147:TYR:CB	0.49	2.61	13	2
1:A:43:GLN:O	1:A:48:LEU:HD12	0.49	2.08	17	1
1:A:15:ALA:CB	1:A:59:ILE:HD11	0.49	2.38	9	2
1:A:12:TRP:CH2	1:A:54:LEU:HD23	0.49	2.42	4	3
1:A:15:ALA:HB1	1:A:62:MET:SD	0.48	2.48	4	1
1:A:182:SER:O	1:A:183:SER:C	0.48	2.52	16	17
1:A:119:GLU:CD	1:A:231:ILE:HG21	0.48	2.28	20	1
1:A:100:LEU:HD21	1:A:180:ASP:N	0.48	2.23	8	1
1:A:61:ILE:CG2	1:A:215:THR:HG23	0.48	2.39	8	3
1:A:157:ALA:HB1	1:A:171:HIS:O	0.48	2.08	19	13
1:A:66:ARG:O	1:A:156:LEU:HD23	0.48	2.08	16	4
1:A:16:GLN:HE22	1:A:35:LEU:HD22	0.48	1.68	14	2
1:A:119:GLU:HG3	1:A:231:ILE:HG21	0.48	1.84	18	1
1:A:100:LEU:HD11	1:A:179:THR:HA	0.47	1.86	15	4
1:A:50:ILE:HD11	1:A:57:ARG:CG	0.47	2.39	13	1
1:A:50:ILE:HD11	1:A:57:ARG:HB3	0.47	1.87	5	1
1:A:97:THR:OG1	1:A:105:VAL:HG21	0.47	2.09	19	8
1:A:113:LEU:HD21	1:A:124:PHE:CD2	0.47	2.44	13	3
1:A:234:ILE:HD11	1:A:238:TYR:CE1	0.47	2.45	19	2
1:A:93:ILE:HG23	1:A:136:ILE:O	0.47	2.09	16	1
1:A:23:TYR:CE2	1:A:72:VAL:HG11	0.47	2.44	5	1
1:A:50:ILE:CD1	1:A:58:VAL:HG23	0.47	2.39	1	4
1:A:193:THR:HG21	1:A:224:PHE:CE1	0.47	2.45	18	2
1:A:23:TYR:HB3	1:A:72:VAL:HG21	0.47	1.86	13	2
1:A:50:ILE:HD12	1:A:58:VAL:CG2	0.47	2.40	11	2
1:A:16:GLN:OE1	1:A:35:LEU:HD21	0.47	2.09	4	1
1:A:111:LYS:HB3	1:A:189:LEU:HD21	0.47	1.87	8	1
1:A:41:GLU:HG3	1:A:42:MET:N	0.47	2.25	18	2
1:A:83:LYS:HD3	1:A:237:LEU:HD13	0.47	1.87	7	3
1:A:44:LYS:HD2	1:A:45:PHE:N	0.46	2.25	5	1
1:A:23:TYR:O	1:A:70:PRO:HB3	0.46	2.11	12	1
1:A:35:LEU:HD11	1:A:39:LEU:HD21	0.46	1.86	14	2
1:A:122:LEU:HD11	1:A:238:TYR:CE1	0.46	2.45	5	1
1:A:20:LYS:HA	1:A:23:TYR:CE1	0.46	2.44	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:GLY:O	1:A:154:ASN:C	0.46	2.54	9	12
1:A:97:THR:HG23	1:A:138:PHE:CE2	0.45	2.46	20	1
1:A:43:GLN:CG	1:A:48:LEU:HD11	0.45	2.41	7	3
1:A:19:LEU:HD11	1:A:42:MET:SD	0.45	2.52	2	1
1:A:119:GLU:OE1	1:A:226:LEU:HD13	0.45	2.11	15	1
1:A:192:ALA:O	1:A:196:LEU:HB2	0.45	2.12	13	10
1:A:83:LYS:CD	1:A:237:LEU:HD23	0.45	2.37	12	1
1:A:83:LYS:HG3	1:A:237:LEU:HD22	0.45	1.89	7	1
1:A:16:GLN:HE22	1:A:35:LEU:HD12	0.45	1.71	15	2
1:A:108:LEU:HD23	1:A:188:PHE:HB3	0.45	1.88	8	1
1:A:58:VAL:O	1:A:61:ILE:CG1	0.44	2.64	8	1
1:A:84:TRP:NE1	1:A:199:SER:O	0.44	2.50	18	2
1:A:43:GLN:HG3	1:A:51:THR:HG22	0.44	1.88	9	2
1:A:88:VAL:HG23	1:A:123:HIS:HD2	0.44	1.72	11	1
1:A:224:PHE:C	1:A:224:PHE:CD1	0.44	2.91	14	2
1:A:154:ASN:O	1:A:155:THR:CB	0.44	2.66	13	5
1:A:94:VAL:HG22	1:A:135:MET:CE	0.44	2.43	12	1
1:A:156:LEU:O	1:A:173:ASP:CB	0.44	2.66	8	1
1:A:68:GLY:HA3	1:A:155:THR:HG22	0.44	1.90	4	1
1:A:91:TYR:O	1:A:127:VAL:CG2	0.44	2.66	19	2
1:A:69:VAL:HG22	1:A:70:PRO:HD2	0.44	1.88	13	1
1:A:193:THR:HG21	1:A:211:VAL:CG2	0.43	2.40	5	1
1:A:58:VAL:O	1:A:61:ILE:HG13	0.43	2.12	20	2
1:A:35:LEU:HD23	1:A:36:GLU:N	0.43	2.28	19	1
1:A:120:ILE:HG21	1:A:234:ILE:CD1	0.43	2.44	7	1
1:A:207:ASP:O	1:A:213:TYR:CD1	0.43	2.71	10	2
1:A:166:LEU:HD13	1:A:166:LEU:N	0.43	2.29	11	2
1:A:107:ARG:HG3	1:A:108:LEU:N	0.43	2.29	17	6
1:A:192:ALA:O	1:A:196:LEU:CD2	0.43	2.65	16	2
1:A:39:LEU:HD11	1:A:54:LEU:CD2	0.43	2.43	19	1
1:A:68:GLY:CA	1:A:155:THR:HG22	0.42	2.45	10	1
1:A:138:PHE:O	1:A:139:ALA:CB	0.42	2.67	4	3
1:A:116:TRP:CZ3	1:A:202:MET:SD	0.42	3.12	20	2
1:A:166:LEU:HD13	1:A:166:LEU:C	0.42	2.35	14	1
1:A:146:SER:O	1:A:147:TYR:CD1	0.42	2.73	13	2
1:A:150:ASP:O	1:A:151:GLY:C	0.42	2.57	11	4
1:A:48:LEU:HD12	1:A:50:ILE:O	0.42	2.14	16	3
1:A:234:ILE:CG1	1:A:238:TYR:CD1	0.42	3.03	15	1
1:A:50:ILE:O	1:A:50:ILE:HD12	0.42	2.14	17	1
1:A:179:THR:HG21	1:A:182:SER:OG	0.42	2.15	6	1
1:A:205:SER:OG	1:A:210:ALA:HB1	0.42	2.13	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLN:HG3	1:A:17:ASP:N	0.42	2.29	4	1
1:A:227:SER:O	1:A:231:ILE:HD12	0.42	2.14	18	2
1:A:166:LEU:HD23	1:A:166:LEU:C	0.42	2.35	9	1
1:A:134:ILE:N	1:A:134:ILE:CD1	0.42	2.80	2	1
1:A:19:LEU:HD13	1:A:19:LEU:C	0.42	2.35	15	1
1:A:122:LEU:HD11	1:A:238:TYR:CE2	0.42	2.50	15	2
1:A:35:LEU:HD21	1:A:39:LEU:HD22	0.42	1.92	7	1
1:A:179:THR:HG21	1:A:182:SER:HB3	0.42	1.91	13	2
1:A:46:PHE:CD1	1:A:61:ILE:HD12	0.42	2.49	17	1
1:A:19:LEU:C	1:A:19:LEU:HD13	0.42	2.36	12	3
1:A:108:LEU:HA	1:A:108:LEU:HD12	0.41	1.76	18	2
1:A:189:LEU:HD12	1:A:224:PHE:CE2	0.41	2.51	12	1
1:A:91:TYR:CD1	1:A:91:TYR:N	0.41	2.88	12	2
1:A:134:ILE:HG22	1:A:136:ILE:HD11	0.41	1.92	18	1
1:A:42:MET:HE2	1:A:61:ILE:HD11	0.41	1.92	15	1
1:A:166:LEU:CD1	1:A:166:LEU:N	0.41	2.83	13	2
1:A:43:GLN:CG	1:A:51:THR:HG22	0.41	2.45	9	1
1:A:90:THR:C	1:A:132:ALA:HB1	0.41	2.35	10	1
1:A:94:VAL:CG2	1:A:135:MET:HB3	0.41	2.45	3	1
1:A:19:LEU:HD13	1:A:38:LYS:CG	0.41	2.46	18	1
1:A:93:ILE:HD11	1:A:109:VAL:HG11	0.41	1.92	8	1
1:A:17:ASP:O	1:A:20:LYS:HG3	0.41	2.15	6	1
1:A:119:GLU:CD	1:A:120:ILE:HG23	0.41	2.36	12	1
1:A:91:TYR:O	1:A:127:VAL:HG21	0.41	2.16	6	2
1:A:35:LEU:HD12	1:A:35:LEU:C	0.41	2.37	2	1
1:A:120:ILE:HD12	1:A:122:LEU:CD1	0.41	2.37	2	1
1:A:20:LYS:HG2	1:A:21:ARG:N	0.41	2.31	14	1
1:A:94:VAL:HG21	1:A:135:MET:HB3	0.40	1.93	6	1
1:A:126:LYS:HE3	1:A:128:VAL:HG13	0.40	1.92	13	1
1:A:149:PHE:C	1:A:151:GLY:N	0.40	2.74	4	1
1:A:43:GLN:HB3	1:A:51:THR:HG22	0.40	1.92	11	1
1:A:16:GLN:CD	1:A:35:LEU:HD13	0.40	2.37	6	1
1:A:101:PRO:HB2	1:A:103:ILE:HG22	0.40	1.93	19	1
1:A:68:GLY:HA3	1:A:155:THR:HG23	0.40	1.90	8	1
1:A:84:TRP:CD1	1:A:162:PRO:HG3	0.40	2.51	15	1
1:A:16:GLN:OE1	1:A:35:LEU:HD12	0.40	2.15	8	1
1:A:113:LEU:HD21	1:A:124:PHE:CE2	0.40	2.51	11	1
1:A:103:ILE:HG23	1:A:104:THR:N	0.40	2.32	10	2
1:A:12:TRP:CE2	1:A:54:LEU:HD23	0.40	2.52	10	1
1:A:110:SER:O	1:A:114:ASN:CB	0.40	2.69	10	1
1:A:227:SER:O	1:A:231:ILE:HG12	0.40	2.17	14	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	201/250 (80%)	173±2 (86±1%)	22±2 (11±1%)	6±2 (3±1%)	9	43
All	All	4020/5000 (80%)	3462 (86%)	440 (11%)	118 (3%)	9	43

All 19 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	55	ASN	20
1	A	147	TYR	20
1	A	224	PHE	18
1	A	122	LEU	15
1	A	151	GLY	7
1	A	154	ASN	6
1	A	50	ILE	6
1	A	139	ALA	4
1	A	144	GLY	4
1	A	164	THR	3
1	A	128	VAL	3
1	A	165	GLY	2
1	A	155	THR	2
1	A	216	TYR	2
1	A	56	SER	2
1	A	66	ARG	1
1	A	202	MET	1
1	A	82	PRO	1
1	A	54	LEU	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	166/208 (80%)	114±4 (69±2%)	52±4 (31±2%)	2	15
All	All	3320/4160 (80%)	2275 (69%)	1045 (31%)	2	15

All 110 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	129	TRP	20
1	A	115	MET	20
1	A	136	ILE	20
1	A	128	VAL	20
1	A	189	LEU	20
1	A	211	VAL	20
1	A	108	LEU	20
1	A	125	ARG	20
1	A	126	LYS	20
1	A	111	LYS	20
1	A	236	LYS	20
1	A	69	VAL	19
1	A	88	VAL	19
1	A	225	LYS	19
1	A	224	PHE	19
1	A	50	ILE	19
1	A	48	LEU	19
1	A	156	LEU	18
1	A	182	SER	18
1	A	113	LEU	18
1	A	207	ASP	18
1	A	205	SER	18
1	A	193	THR	17
1	A	36	GLU	16
1	A	131	THR	16
1	A	215	THR	15
1	A	200	LEU	15
1	A	199	SER	15
1	A	174	GLU	15
1	A	16	GLN	14
1	A	86	SER	14
1	A	72	VAL	14
1	A	155	THR	14
1	A	67	CYS	14
1	A	150	ASP	13
1	A	38	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	147	TYR	11
1	A	59	ILE	11
1	A	145	ASP	10
1	A	164	THR	10
1	A	149	PHE	10
1	A	232	LYS	10
1	A	64	LYS	10
1	A	66	ARG	9
1	A	85	THR	9
1	A	180	ASP	9
1	A	100	LEU	9
1	A	55	ASN	9
1	A	99	ASP	9
1	A	97	THR	9
1	A	87	LYS	9
1	A	175	ASP	9
1	A	119	GLU	9
1	A	98	ARG	8
1	A	61	ILE	8
1	A	21	ARG	8
1	A	229	ASP	7
1	A	71	ASP	7
1	A	184	LEU	7
1	A	212	MET	7
1	A	226	LEU	7
1	A	227	SER	7
1	A	107	ARG	7
1	A	146	SER	7
1	A	60	GLU	7
1	A	17	ASP	6
1	A	20	LYS	6
1	A	202	MET	6
1	A	118	LYS	6
1	A	39	LEU	6
1	A	57	ARG	6
1	A	213	TYR	6
1	A	166	LEU	6
1	A	35	LEU	5
1	A	190	TYR	5
1	A	40	LYS	5
1	A	83	LYS	5
1	A	140	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	53	MET	5
1	A	95	SER	5
1	A	230	ASP	5
1	A	14	GLN	5
1	A	216	TYR	4
1	A	19	LEU	4
1	A	106	ASP	4
1	A	92	ARG	4
1	A	42	MET	4
1	A	133	ASP	4
1	A	103	ILE	4
1	A	235	GLN	4
1	A	206	SER	4
1	A	187	ASN	4
1	A	90	THR	4
1	A	22	PHE	3
1	A	154	ASN	3
1	A	228	GLN	3
1	A	177	ARG	3
1	A	18	TYR	3
1	A	209	ASN	2
1	A	62	MET	2
1	A	51	THR	2
1	A	135	MET	2
1	A	41	GLU	2
1	A	169	ASP	1
1	A	176	GLU	1
1	A	234	ILE	1
1	A	237	LEU	1
1	A	44	LYS	1
1	A	188	PHE	1
1	A	56	SER	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 [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: 2mze_cs.str

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	2659
Number of shifts mapped to atoms	2659
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	236	-0.28 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	212	0.27 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	231	0.04 ± 0.10	None needed (< 0.5 ppm)
^{15}N	218	-0.16 ± 0.28	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 83%, i.e. 2043 atoms were assigned a chemical shift out of a possible 2469. 25 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	950/983 (97%)	373/391 (95%)	392/402 (98%)	185/190 (97%)
Sidechain	915/1208 (76%)	565/713 (79%)	342/444 (77%)	8/51 (16%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	178/278 (64%)	91/148 (61%)	82/117 (70%)	5/13 (38%)
Overall	2043/2469 (83%)	1029/1252 (82%)	816/963 (85%)	198/254 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 2380 atoms were assigned a chemical shift out of a possible 3056. 27 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1129/1220 (93%)	444/485 (92%)	467/500 (93%)	218/235 (93%)
Sidechain	1049/1533 (68%)	646/908 (71%)	394/555 (71%)	9/70 (13%)
Aromatic	202/303 (67%)	103/161 (64%)	94/129 (73%)	5/13 (38%)
Overall	2380/3056 (78%)	1193/1554 (77%)	955/1184 (81%)	232/318 (73%)

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	107	ARG	NE	119.85	92.63 – 76.73	22.1
1	A	92	ARG	NE	117.04	92.63 – 76.73	20.4
1	A	60	GLU	HB2	0.60	3.08 – 0.98	-6.8
1	A	22	PHE	CE2	122.89	136.81 – 124.71	-6.5
1	A	162	PRO	HB3	-0.32	3.81 – 0.21	-6.5
1	A	60	GLU	HB3	0.64	3.10 – 0.90	-6.2
1	A	65	PRO	HA	2.44	6.05 – 2.75	-6.0
1	A	22	PHE	CE1	122.89	137.92 – 123.42	-5.4
1	A	62	MET	HG3	0.38	4.30 – 0.50	-5.3

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:

