WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 12:48 PM EST

PDB ID	:	1Q5W
Title	:	Ubiquitin Recognition by Npl4 Zinc-Fingers
Authors	:	Alam, S.L.; Sun, J.; Payne, M.; Welch, B.D.; Blake, B.K.; Davis, D.R.; Meyer, H.H.; Emr, S.D.; Sundquist, W.I.
Deposited on	:	2003-08-11

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
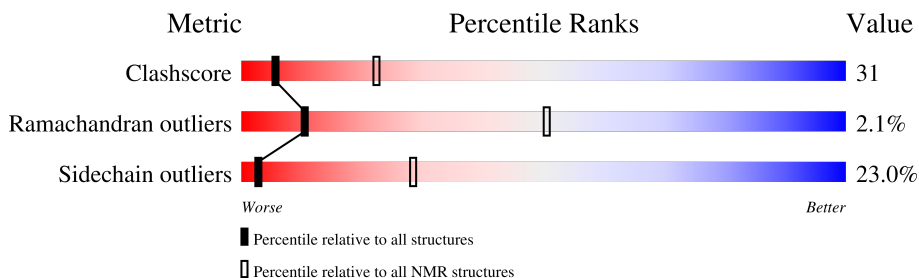with specific help available everywhere you see the (i) symbol.

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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 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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		2.1%
Sidechain outliers		23.0%

Worse — *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	31	29% 52% • 16%
2	B	76	42% 46% 7% 5%

2   Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations,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:6-A:31, B:101-B:172 (98)	0.23	14

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1671 atoms, of which 838 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called homolog of yeast nuclear protein localization 4.

Mol	Chain	Residues	Atoms						Trace
1	A	31	Total	C	H	N	O	S	0
			438	137	208	42	44	7	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9ES54
A	2	SER	-	cloning artifact	UNP Q9ES54

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			1232	378	630	105	118	1	

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

| Mol	Chain	Residues	Atoms	
3	A	1	Total	Zn
			1	1

4 Residue-property plots ⓘ

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: homolog of yeast nuclear protein localization 4

Chain A:

29%   52%   •   16%

- Molecule 2: Ubiquitin

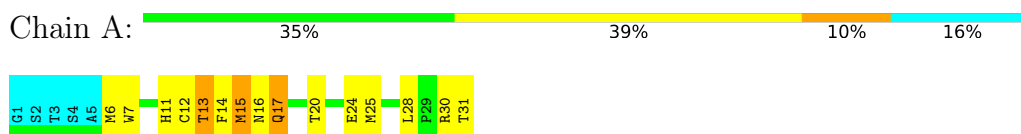Chain B:

42%   46%   7%   5%
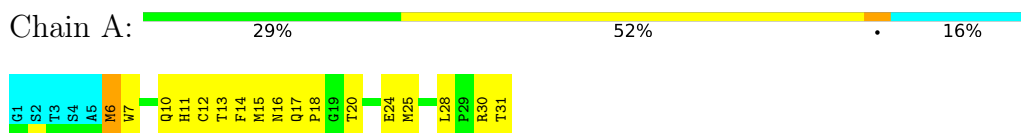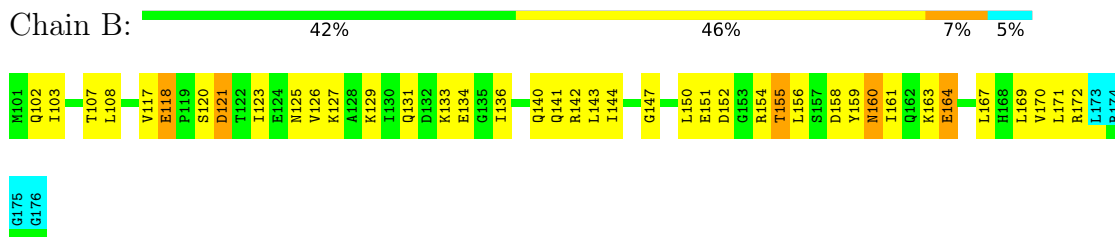
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

35%   39%   10%   16%

- Molecule 2: Ubiquitin

Chain B:

46%   42%   7% 5%

M101 Q102 I103 F104 L108 K111 T112 I113 T114 L115 E116 V117 E118 P119 S120 D121 T122 I123 V126 K129 I130 Q131 D132 K133 I136 Q140 Q141 R142 L143 G147 L150 E151 R154 T155 L156 S157 D158 Y159 N160 I161 Q162 K163 E164 L167 H168 L169 V170 L171 R172 L173

R174 G175 G176

4.2.2　Score per residue for model 2

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:　45%　　29%　　10%　　16%

G1 S2 T3 S4 A5 M6 W7 H11 C12 T13 F14 M15 N16 Q17 T20 M25 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B:　53%　　36%　　7%　5%

M101 Q102 I103 T107 V117 E118 P119 S120 D121 T122 I123 V126 K127 A128 K129 I130 Q131 D132 K133 I136 Q141 R142 L143 G147 L150 E151 D152 G153 R154 T155 L156 S157 D158 Y159 N160 I161 Q162 K163 E164 L167 H168 L169 V170 L171 R172 L173 R174 G175 G176

4.2.3　Score per residue for model 3

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:　35%　　42%　　6%　　16%

G1 S2 T3 S4 A5 M6 W7 Q10 H11 C12 T13 F14 M15 N16 Q17 T20 M25 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B:　42%　　45%　　8%　5%

M101 Q102 I103 F104 V105 K106 T107 L108 I113 T114 L115 E116 V117 E118 P119 S120 D121 T122 I123 E124 M125 V126 Q131 D132 K133 I136 Q140 Q141 R142 L143 I144 Q149 L150 E151 R154 T155 L156 S157 D158 Y159 N160 I161 Q162 K163 E164 L167 H168 L169 V170 L171 R172 L173 R174

G175 G176
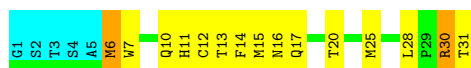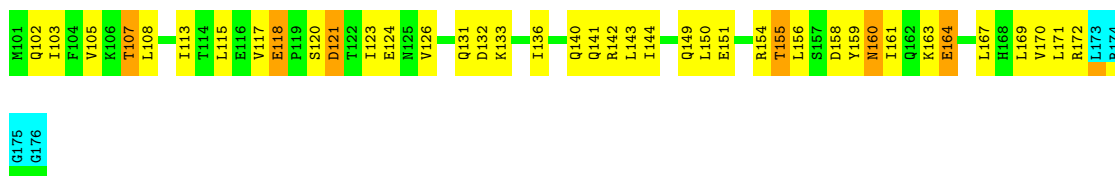
4.2.4　Score per residue for model 4

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:　32%　　45%　　6%　　16%

G1 S2 T3 S4 A5 M6 W7 H11 C12 T13 F14 M15 N16 Q17 P18 G19 T20 G21 H22 C23 E24 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B: 42% 45% 8% 5%

M101 Q102 I103 T107 L108 I113 T114 L115 E116 V117 E118 P119 S120 D121 V126 K127 A128 K129 I130 Q131 D132 K133 E134 G135 I136 D139 Q140 Q141 R142 L143 I144 G147 L150 E151 R154 T155 L156 S157 D158 Y159 N160 I161 E164 L167 H168 L169 V170 L171 R172 L173 R174

G175 G176
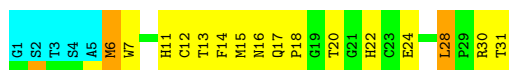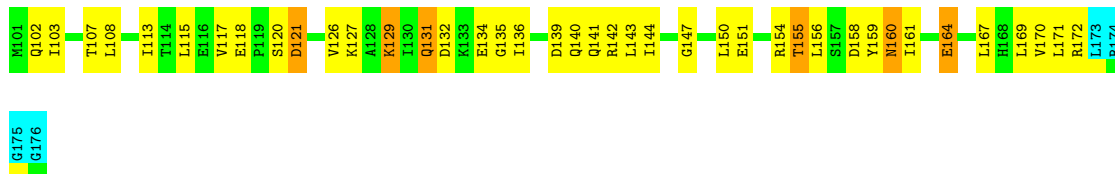
4.2.5 Score per residue for model 5

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A: 35% 45% • 16%

G1 S2 T3 S4 A5 M6 W7 H11 C12 T13 F14 M15 N16 Q17 P18 G19 T20 M25 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B: 41% 45% 9% 5%

M101 Q102 I103 T107 L108 T109 V117 E118 P119 S120 D121 N125 V126 K127 Q131 D132 K133 E134 G135 I136 Q140 Q141 R142 L143 I144 F145 L150 E151 D152 G153 R154 T155 L156 S157 D158 Y159 N160 I161 Q162 K163 E164 L167 H168 L169 V170 L171 R172 L173 R174 G175 G176
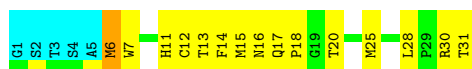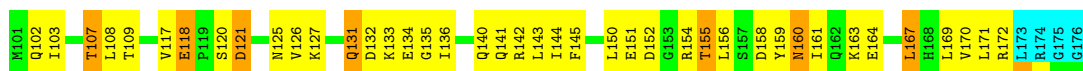
4.2.6 Score per residue for model 6

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A: 35% 39% 10% 16%

G1 S2 T3 S4 A5 M6 W7 H11 C12 T13 F14 M15 N16 Q17 P18 G19 T20 M25 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B: 45% 42% 8% 5%

M101 Q102 I103 T107 I113 V117 E118 P119 S120 D121 T122 I123 E124 N125 V126 K129 I130 Q131 D132 K133 E134 G135 I136 Q140 Q141 R142 G147 L150 E151 D152 G153 R154 T155 L156 S157 D158 Y159 N160 I161 Q162 K163 E164 L167 H168 L169 V170 L171 R172 L173 R174 G175 G176
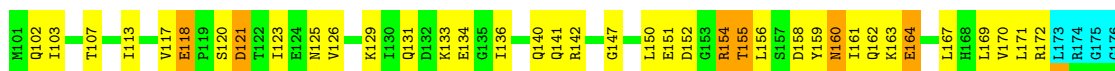
4.2.7　Score per residue for model 7

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

• Molecule 2: Ubiquitin

Chain B:

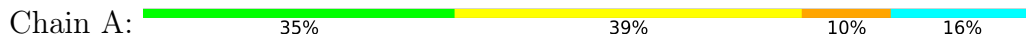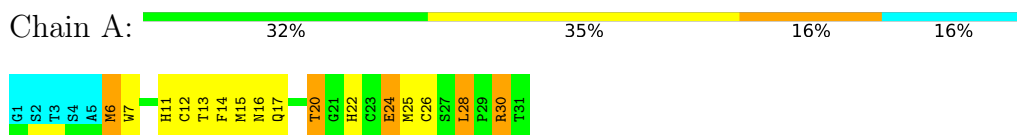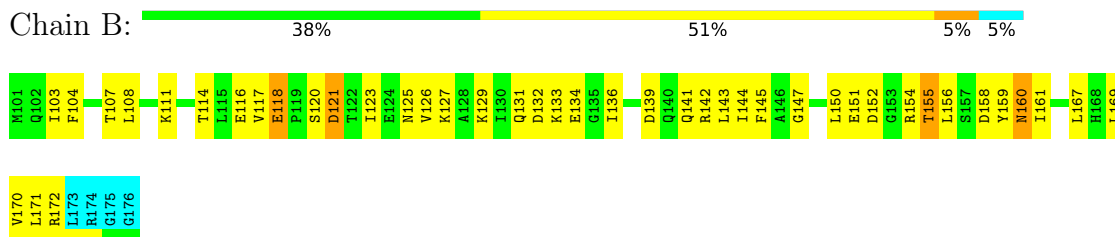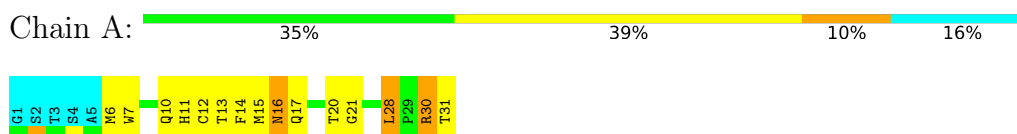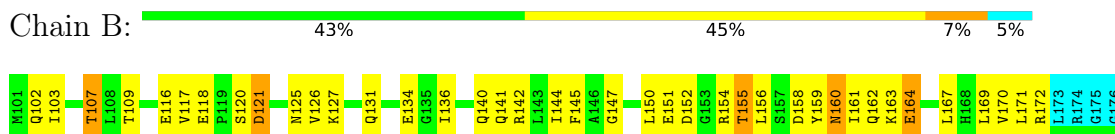#### 4.2.8　Score per residue for model 8

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

• Molecule 2: Ubiquitin

Chain B:

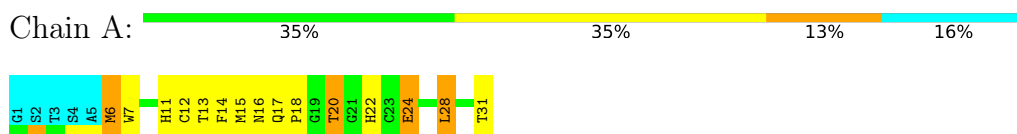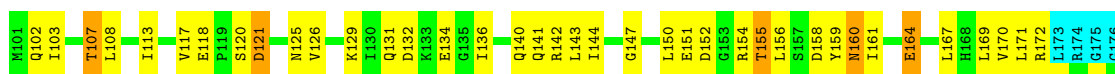#### 4.2.9　Score per residue for model 9

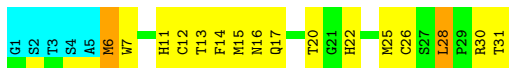• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

• Molecule 2: Ubiquitin

Chain B:

M101 Q102 I103 T107 L108 I113 V117 E118 P119 S120 D121 N125 V126 K129 I130 Q131 D132 K133 E134 G135 I136 Q140 Q141 R142 L143 I144 G147 L150 E151 D152 G153 R154 T155 L156 S157 D158 Y159 N160 I161 E164 L167 H168 L169 V170 L171 R172 L173 R174 G175 G176

4.2.10 Score per residue for model 10

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A: 32% 45% 6% 16%

G1 S2 T3 S4 A5 M6 W7 H11 C12 T13 F14 M15 N16 Q17 T20 G21 H22 M25 C26 S27 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B: 43% 46% 5% 5%

M101 Q102 I103 F104 T107 L108 T114 V117 E118 P119 S120 D121 T122 I123 E124 N125 V126 K127 Q131 D132 K133 E134 G135 I136 Q140 Q141 R142 L143 I144 F145 A146 G147 K148 Q149 L150 E151 D152 G153 R154 T155 L156 S157 D158 Y159 N160 I161 E164 L167 H168 L169 V170 L171 R172

L173 R174 G175 G176
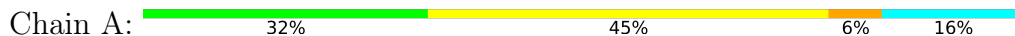
4.2.11 Score per residue for model 11

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A: 29% 42% 13% 16%

G1 S2 T3 S4 A5 M6 W7 Q10 H11 C12 T13 F14 M15 N16 Q17 P18 G19 T20 M25 C26 S27 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B: 43% 46% 5% 5%

M101 Q102 I103 T107 L108 V117 E118 P119 S120 D121 T122 I123 E124 N125 V126 K127 A128 K129 I130 Q131 D132 K133 E134 G135 I136 D139 Q140 Q141 R142 L143 I144 L150 E151 R154 T155 L156 S157 D158 Y159 N160 I161 Q162 K163 E164 L167 H168 L169 V170 L171 R172 L173 R174 G175 G176

4.2.12 Score per residue for model 12

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A: 23% 55% 6% 16%

G1 S2 T3 S4 A5 M6 W7 A8 C9 Q10 H11 C12 T13 F14 M15 N16 Q17 P18 G19 T20 G21 H22 C23 E24 M25 L28 P29 R30 T31

• Molecule 2: Ubiquitin

Chain B:

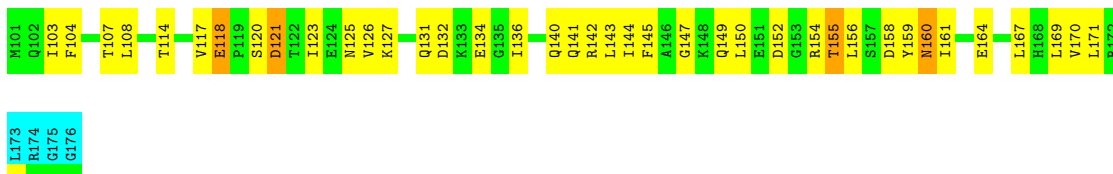### 4.2.13 Score per residue for model 13

• Molecule 1: homolog of yeast nuclear protein localization 4
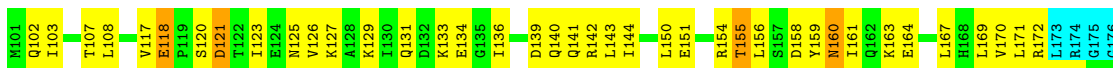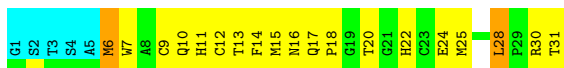
Chain A:

• Molecule 2: Ubiquitin

Chain B:

4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

• Molecule 2: Ubiquitin

Chain B:
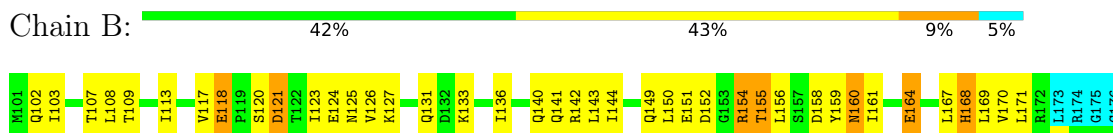
4.2.15 Score per residue for model 15

• Molecule 1: homolog of yeast nuclear protein localization 4
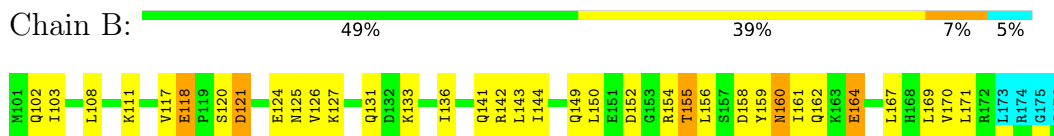
Chain A:

• Molecule 2: Ubiquitin

Chain B:
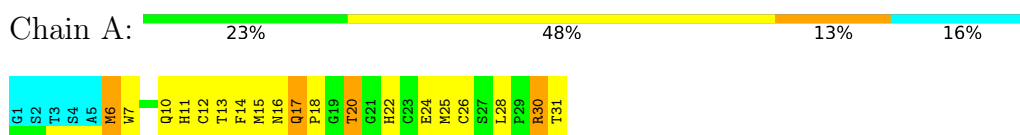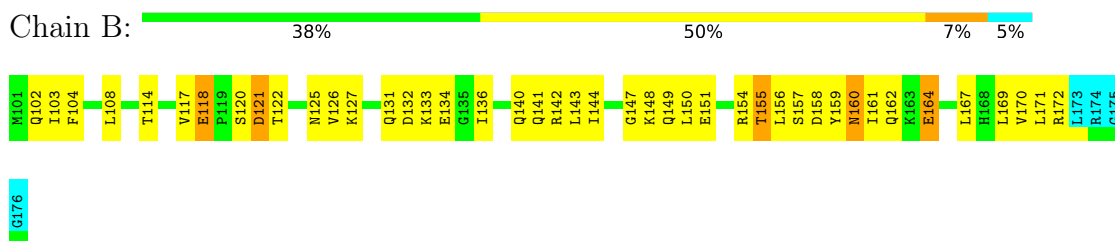
4.2.16 Score per residue for model 16

• Molecule 1: homolog of yeast nuclear protein localization 4
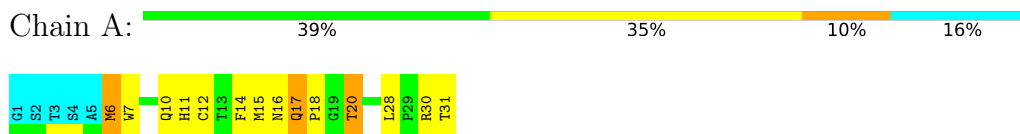
Chain A:

• Molecule 2: Ubiquitin

Chain B:
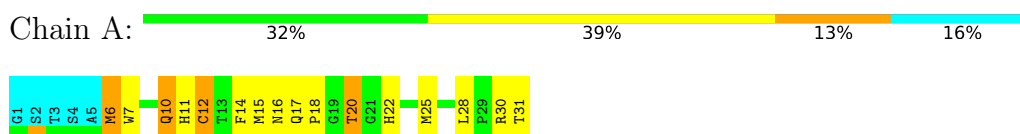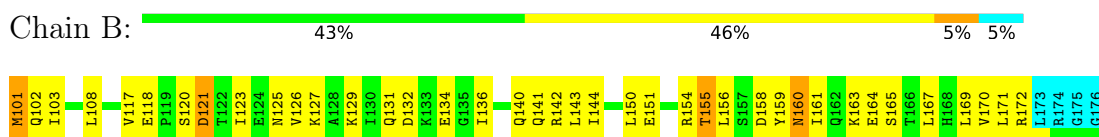
4.2.17 Score per residue for model 17

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

• Molecule 2: Ubiquitin

Chain B:
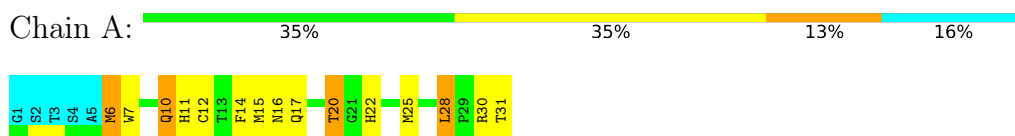
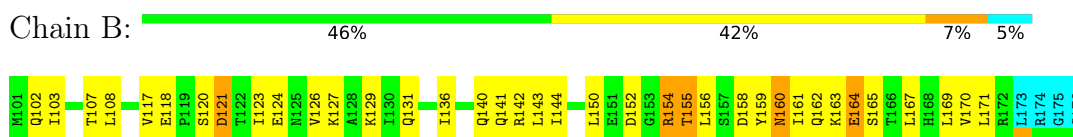#### 4.2.18　Score per residue for model 18

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

• Molecule 2: Ubiquitin

Chain B:
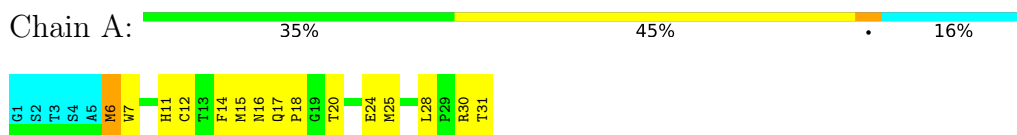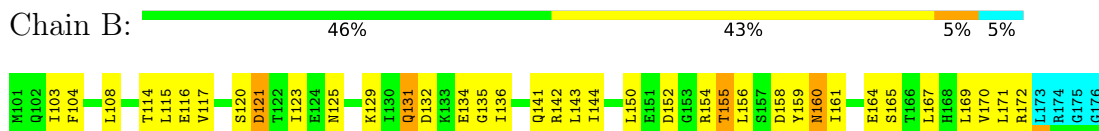
4.2.19　Score per residue for model 19

• Molecule 1: homolog of yeast nuclear protein localization 4

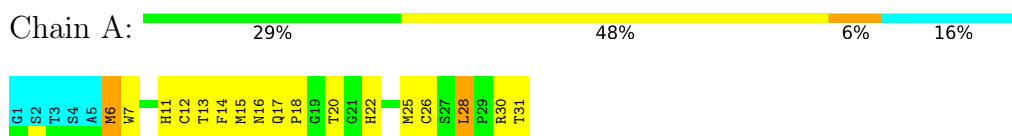Chain A:

• Molecule 2: Ubiquitin

Chain B:
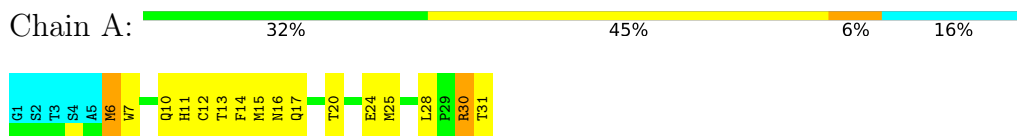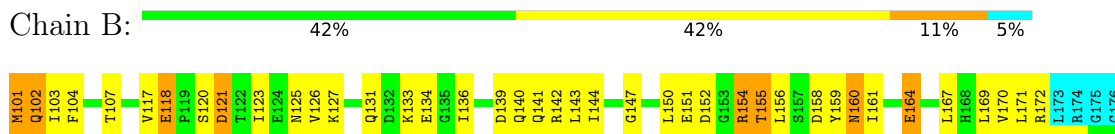
4.2.20　Score per residue for model 20

• Molecule 1: homolog of yeast nuclear protein localization 4

Chain A:

• Molecule 2: Ubiquitin

Chain B:
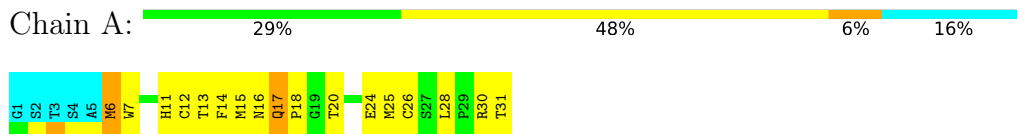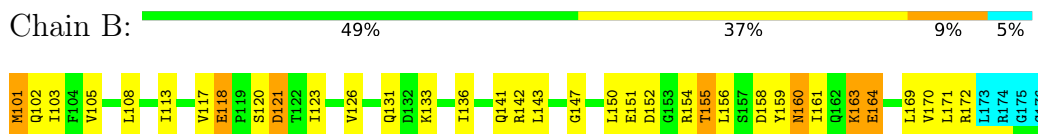
5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *Torsion angle dynamics followed by simulated annealing.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations,structures with the lowest energy,target function.*

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

Software name	Classification	Version
DYANA	refinement	1.5
CNS	refinement	1.1

No chemical shift data was provided.

6   Model quality (i)

6.1   Standard geometry (i)

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

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	202	181	179	21±3
2	B	574	600	596	32±5
All	All	15540	15620	15500	953

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:136:ILE:HD13	2:B:169:LEU:HD21	0.86	1.45	19	7
2:B:156:LEU:HD22	2:B:161:ILE:HG21	0.85	1.47	4	19
1:A:11:HIS:CD2	1:A:28:LEU:HD22	0.85	2.06	12	9
1:A:14:PHE:HB2	2:B:144:ILE:HD12	0.85	1.48	17	9
2:B:117:VAL:HG11	2:B:126:VAL:HG22	0.83	1.47	3	13
2:B:121:ASP:O	2:B:155:THR:HG22	0.78	1.78	3	20
2:B:156:LEU:HD23	2:B:161:ILE:HD13	0.78	1.56	17	17
1:A:11:HIS:CD2	1:A:28:LEU:HD23	0.77	2.15	13	11
2:B:136:ILE:CG2	2:B:171:LEU:HD21	0.77	2.10	20	19
2:B:118:GLU:O	2:B:156:LEU:HD12	0.76	1.80	3	18
2:B:136:ILE:HG23	2:B:171:LEU:HD21	0.75	1.57	10	19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:156:LEU:CD2	2:B:161:ILE:HD13	0.75	2.11	7	15
2:B:101:MET:SD	2:B:117:VAL:HG23	0.75	2.21	16	4
2:B:136:ILE:CD1	2:B:169:LEU:HD21	0.74	2.12	14	15
2:B:141:GLN:HG2	2:B:169:LEU:HD11	0.73	1.60	13	19
2:B:150:LEU:HD11	2:B:167:LEU:CD2	0.71	2.16	18	8
2:B:156:LEU:HD22	2:B:161:ILE:CG2	0.70	2.16	4	4
2:B:103:ILE:HD11	2:B:126:VAL:HG13	0.70	1.63	1	16
2:B:103:ILE:HD11	2:B:126:VAL:CG1	0.70	2.17	10	19
2:B:117:VAL:CG1	2:B:126:VAL:HG22	0.69	2.18	14	6
1:A:26:CYS:HB3	2:B:108:LEU:HD11	0.68	1.65	10	6
2:B:145:PHE:CB	2:B:150:LEU:HD21	0.66	2.19	8	1
1:A:14:PHE:CD1	2:B:144:ILE:HD12	0.66	2.26	4	7
1:A:14:PHE:CB	2:B:144:ILE:HD12	0.66	2.21	18	9
2:B:156:LEU:HD23	2:B:161:ILE:CD1	0.65	2.21	19	2
2:B:107:THR:HG22	2:B:169:LEU:HD23	0.65	1.69	14	7
2:B:123:ILE:CG2	2:B:143:LEU:HD12	0.65	2.22	19	11
2:B:141:GLN:CG	2:B:169:LEU:HD11	0.64	2.22	5	5
2:B:143:LEU:CB	2:B:150:LEU:HD12	0.64	2.22	15	5
1:A:7:TRP:CE2	1:A:16:ASN:HB2	0.64	2.27	1	20
2:B:136:ILE:HD12	2:B:169:LEU:HD21	0.62	1.70	12	8
2:B:150:LEU:HD11	2:B:167:LEU:HD23	0.62	1.70	15	1
2:B:107:THR:CG2	2:B:169:LEU:HD23	0.61	2.25	8	7
2:B:145:PHE:HB3	2:B:150:LEU:HD21	0.61	1.73	7	3
2:B:141:GLN:OE1	2:B:169:LEU:HD13	0.60	1.96	14	5
2:B:103:ILE:HG23	2:B:117:VAL:CG2	0.60	2.26	19	17
2:B:108:LEU:HG	2:B:170:VAL:HG22	0.60	1.73	3	10
1:A:6:MET:HB2	1:A:15:MET:HE1	0.60	1.74	10	8
2:B:123:ILE:HG23	2:B:143:LEU:HD12	0.59	1.74	14	10
2:B:140:GLN:OE1	2:B:171:LEU:HD22	0.59	1.97	8	7
1:A:12:CYS:HB3	2:B:108:LEU:HD11	0.58	1.76	1	2
1:A:10:GLN:OE1	1:A:31:THR:HG22	0.58	1.98	8	1
2:B:140:GLN:OE1	2:B:171:LEU:HD13	0.58	1.99	8	1
1:A:12:CYS:CB	2:B:108:LEU:HD21	0.58	2.28	17	13
1:A:14:PHE:CG	2:B:144:ILE:HD12	0.58	2.34	19	4
2:B:143:LEU:HB3	2:B:150:LEU:HD12	0.57	1.77	12	6
1:A:12:CYS:CA	2:B:108:LEU:HD21	0.57	2.30	3	8
2:B:103:ILE:HD11	2:B:126:VAL:HG11	0.57	1.76	14	5
2:B:156:LEU:HD22	2:B:161:ILE:CB	0.56	2.30	9	3
2:B:115:LEU:HD22	2:B:129:LYS:HD3	0.56	1.75	18	1
1:A:11:HIS:CG	1:A:28:LEU:HD23	0.55	2.36	20	7
1:A:12:CYS:HB2	2:B:170:VAL:HG21	0.55	1.78	3	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:10:GLN:CD	1:A:31:THR:HG22	0.55	2.22	13	3
2:B:150:LEU:HD11	2:B:167:LEU:HD21	0.55	1.78	6	1
1:A:13:THR:O	2:B:144:ILE:HG21	0.55	2.01	12	4
1:A:26:CYS:CB	2:B:108:LEU:HD11	0.55	2.31	10	2
1:A:20:THR:HG21	1:A:24:GLU:OE2	0.55	2.01	9	1
1:A:17:GLN:HB3	1:A:18:PRO:CD	0.54	2.33	20	8
1:A:14:PHE:HD1	2:B:144:ILE:HD12	0.54	1.60	8	3
1:A:7:TRP:CD1	1:A:17:GLN:O	0.54	2.61	20	20
1:A:7:TRP:CE2	1:A:16:ASN:CB	0.54	2.91	19	19
1:A:11:HIS:NE2	1:A:28:LEU:HD22	0.53	2.18	4	6
2:B:136:ILE:HG22	2:B:141:GLN:HG3	0.53	1.81	17	13
2:B:127:LYS:HE3	2:B:143:LEU:HD12	0.53	1.80	5	1
1:A:22:HIS:HB3	1:A:28:LEU:O	0.53	2.04	9	9
1:A:7:TRP:CZ3	1:A:16:ASN:ND2	0.52	2.78	1	18
1:A:15:MET:HE3	1:A:15:MET:HA	0.52	1.81	2	2
2:B:159:TYR:O	2:B:160:ASN:HB3	0.52	2.05	8	20
1:A:25:MET:C	2:B:170:VAL:HG11	0.52	2.25	15	3
2:B:115:LEU:HD22	2:B:129:LYS:HG2	0.52	1.82	1	2
2:B:143:LEU:HD13	2:B:150:LEU:HD12	0.52	1.82	14	5
1:A:6:MET:HB3	1:A:16:ASN:O	0.51	2.05	16	9
2:B:127:LYS:CE	2:B:143:LEU:HD12	0.51	2.35	5	1
2:B:150:LEU:HD11	2:B:167:LEU:HD22	0.51	1.82	13	2
2:B:150:LEU:HD22	2:B:159:TYR:CG	0.51	2.40	20	1
2:B:150:LEU:CD1	2:B:167:LEU:HD23	0.51	2.35	4	4
1:A:20:THR:HG21	1:A:24:GLU:OE1	0.51	2.05	7	2
2:B:107:THR:OG1	2:B:109:THR:HG22	0.50	2.06	14	1
2:B:104:PHE:CE1	2:B:114:THR:HG23	0.50	2.42	10	3
1:A:20:THR:HG21	1:A:24:GLU:CD	0.50	2.26	9	2
1:A:6:MET:CB	1:A:15:MET:HE1	0.49	2.37	7	8
1:A:28:LEU:CD1	1:A:28:LEU:N	0.49	2.76	8	11
1:A:11:HIS:CD2	1:A:28:LEU:CD2	0.48	2.95	18	12
2:B:150:LEU:HD23	2:B:159:TYR:CE2	0.48	2.44	7	3
2:B:103:ILE:CD1	2:B:126:VAL:HG11	0.48	2.39	10	7
1:A:6:MET:HE3	1:A:15:MET:SD	0.48	2.49	3	2
2:B:156:LEU:CD2	2:B:161:ILE:HG21	0.48	2.37	18	2
1:A:15:MET:CG	2:B:147:GLY:CA	0.47	2.93	2	2
2:B:102:GLN:O	2:B:164:GLU:N	0.47	2.48	20	15
2:B:145:PHE:HB2	2:B:167:LEU:HD23	0.47	1.85	5	1
1:A:12:CYS:CB	2:B:170:VAL:HG21	0.47	2.39	8	9
1:A:14:PHE:CD2	1:A:25:MET:CG	0.47	2.98	19	11
1:A:6:MET:HE2	1:A:15:MET:CE	0.47	2.39	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:MET:HB2	2:B:147:GLY:O	0.47	2.09	10	2
2:B:150:LEU:HD22	2:B:159:TYR:CD2	0.46	2.45	20	1
1:A:14:PHE:CZ	1:A:25:MET:CE	0.46	2.99	18	1
2:B:136:ILE:HD13	2:B:169:LEU:CD2	0.46	2.31	19	1
1:A:7:TRP:N	1:A:15:MET:HE1	0.46	2.26	1	3
2:B:145:PHE:HB2	2:B:150:LEU:HD21	0.46	1.87	8	1
2:B:159:TYR:O	2:B:160:ASN:CB	0.46	2.64	19	18
2:B:150:LEU:CD2	2:B:159:TYR:CD2	0.46	2.99	7	4
1:A:30:ARG:O	1:A:31:THR:HG22	0.46	2.10	12	13
1:A:7:TRP:O	1:A:16:ASN:OD1	0.46	2.34	8	1
1:A:15:MET:HG2	2:B:147:GLY:CA	0.45	2.41	20	2
2:B:167:LEU:N	2:B:167:LEU:HD12	0.45	2.25	12	9
1:A:15:MET:HE3	1:A:15:MET:CA	0.45	2.42	1	2
1:A:7:TRP:CH2	1:A:16:ASN:ND2	0.45	2.84	7	4
2:B:150:LEU:CD2	2:B:161:ILE:HD11	0.45	2.40	2	2
2:B:154:ARG:CZ	2:B:159:TYR:CE2	0.45	3.00	2	2
2:B:154:ARG:NE	2:B:159:TYR:CE2	0.45	2.85	14	3
2:B:150:LEU:CD2	2:B:159:TYR:CG	0.45	3.00	17	4
1:A:20:THR:HG22	1:A:22:HIS:O	0.45	2.11	16	3
2:B:154:ARG:CZ	2:B:159:TYR:CZ	0.45	3.00	13	1
1:A:7:TRP:CZ2	1:A:30:ARG:HB2	0.45	2.47	19	7
1:A:25:MET:HE2	2:B:149:GLN:HB3	0.45	1.88	14	2
2:B:103:ILE:HD13	2:B:117:VAL:HG21	0.45	1.89	13	2
2:B:150:LEU:HD23	2:B:159:TYR:CD2	0.44	2.47	15	1
1:A:14:PHE:CG	1:A:15:MET:N	0.44	2.84	13	4
1:A:14:PHE:CE1	1:A:25:MET:CE	0.44	3.00	1	1
2:B:117:VAL:HG11	2:B:126:VAL:CG2	0.44	2.32	14	1
1:A:12:CYS:HA	2:B:108:LEU:HD21	0.44	1.88	3	5
1:A:12:CYS:C	1:A:13:THR:HG23	0.44	2.32	7	3
2:B:143:LEU:CD1	2:B:150:LEU:HD12	0.44	2.43	13	1
2:B:105:VAL:HG21	2:B:115:LEU:HD12	0.44	1.89	3	1
2:B:123:ILE:HG23	2:B:143:LEU:CD1	0.44	2.42	18	2
1:A:12:CYS:HB2	2:B:170:VAL:CG2	0.44	2.42	15	1
2:B:143:LEU:HB2	2:B:150:LEU:HD12	0.43	1.89	15	1
2:B:116:GLU:O	2:B:116:GLU:CG	0.43	2.66	7	3
1:A:7:TRP:CH2	1:A:16:ASN:OD1	0.43	2.72	12	1
1:A:7:TRP:CE3	1:A:16:ASN:OD1	0.43	2.71	8	1
1:A:10:GLN:CG	1:A:11:HIS:CE1	0.43	3.01	16	2
2:B:103:ILE:CG2	2:B:117:VAL:CG2	0.43	2.97	20	5
1:A:6:MET:CE	1:A:15:MET:CE	0.43	2.97	3	9
2:B:104:PHE:CD1	2:B:114:THR:HG23	0.43	2.49	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:14:PHE:CD2	1:A:25:MET:HG2	0.43	2.48	7	5
2:B:107:THR:HB	2:B:109:THR:HG22	0.43	1.91	8	2
1:A:15:MET:HG2	2:B:147:GLY:HA3	0.42	1.91	9	4
2:B:156:LEU:O	2:B:161:ILE:HD13	0.42	2.14	13	1
1:A:15:MET:HG3	2:B:147:GLY:HA3	0.42	1.89	19	1
2:B:163:LYS:N	2:B:163:LYS:CD	0.42	2.81	20	1
1:A:21:GLY:O	1:A:30:ARG:HB3	0.42	2.15	8	1
1:A:15:MET:HG3	2:B:147:GLY:CA	0.42	2.44	19	1
2:B:150:LEU:HD21	2:B:161:ILE:HD11	0.42	1.92	2	1
2:B:105:VAL:N	2:B:113:ILE:O	0.42	2.53	17	2
1:A:14:PHE:CZ	1:A:25:MET:HE3	0.42	2.49	18	1
1:A:6:MET:CE	1:A:15:MET:SD	0.42	3.08	18	8
1:A:14:PHE:CG	1:A:25:MET:HG3	0.42	2.49	15	3
1:A:10:GLN:HG2	1:A:11:HIS:CE1	0.42	2.50	17	6
2:B:131:GLN:O	2:B:135:GLY:N	0.42	2.52	5	3
1:A:17:GLN:CD	1:A:17:GLN:N	0.42	2.73	20	2
1:A:15:MET:CA	1:A:15:MET:CE	0.41	2.98	8	4
1:A:14:PHE:CD1	1:A:25:MET:HG3	0.41	2.50	2	3
2:B:103:ILE:CD1	2:B:126:VAL:CG1	0.41	2.99	16	6
1:A:25:MET:CE	2:B:149:GLN:NE2	0.41	2.83	15	1
2:B:123:ILE:HD12	2:B:150:LEU:HD13	0.41	1.90	6	2
1:A:20:THR:H	1:A:20:THR:HG1	0.41	1.49	13	1
1:A:7:TRP:CH2	1:A:30:ARG:HB2	0.41	2.50	6	8
1:A:30:ARG:O	1:A:31:THR:CG2	0.41	2.68	12	1
1:A:12:CYS:O	1:A:13:THR:CB	0.41	2.69	1	1
2:B:150:LEU:CD1	2:B:167:LEU:CD2	0.41	2.99	1	2
2:B:154:ARG:NE	2:B:159:TYR:CE1	0.41	2.89	6	1
1:A:12:CYS:HB3	2:B:108:LEU:HD21	0.41	1.93	17	1
2:B:150:LEU:HD23	2:B:159:TYR:CG	0.41	2.51	6	1
1:A:13:THR:OG1	2:B:168:HIS:CD2	0.41	2.74	14	1
2:B:167:LEU:HD12	2:B:167:LEU:N	0.40	2.31	7	1
2:B:168:HIS:ND1	2:B:168:HIS:N	0.40	2.69	14	1
1:A:14:PHE:CD2	1:A:25:MET:HG3	0.40	2.51	15	1
2:B:104:PHE:CD2	2:B:165:SER:O	0.40	2.74	18	1
2:B:104:PHE:CE1	2:B:164:GLU:OE1	0.40	2.75	17	3
1:A:17:GLN:HB3	1:A:18:PRO:HD2	0.40	1.93	13	1
1:A:7:TRP:CZ3	1:A:16:ASN:OD1	0.40	2.74	8	1
1:A:14:PHE:HA	2:B:144:ILE:HG21	0.40	1.92	8	1
1:A:14:PHE:HA	2:B:144:ILE:CG2	0.40	2.47	10	1
2:B:103:ILE:HG23	2:B:117:VAL:HG22	0.40	1.93	18	1

6.3   Torsion angles ⓘ

6.3.1   Protein backbone ⓘ

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	25/31 (81%)	21±1 (84±4%)	4±1 (16±4%)	0±0 (0±1%)	50	82
2	B	71/76 (93%)	67±1 (94±1%)	2±1 (3±1%)	2±0 (3±0%)	8	42
All	All	1920/2140 (90%)	1754 (91%)	125 (7%)	41 (2%)	10	50

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	121	ASP	20
2	B	160	ASN	20
1	A	9	CYS	1

6.3.2   Protein sidechains ⓘ

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	23/26 (88%)	18±1 (80±4%)	4±1 (20±4%)	4	34
2	B	66/68 (97%)	50±2 (76±3%)	16±2 (24±3%)	2	26
All	All	1780/1880 (95%)	1370 (77%)	410 (23%)	3	28

All 47 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	6	MET	20
1	A	20	THR	20
2	B	120	SER	20
2	B	131	GLN	20

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Mol	Chain	Res	Type	Models (Total)
2	B	154	ARG	20
2	B	155	THR	20
2	B	158	ASP	20
2	B	142	ARG	19
2	B	164	GLU	16
2	B	151	GLU	15
2	B	172	ARG	15
2	B	125	ASN	14
2	B	118	GLU	13
2	B	133	LYS	13
2	B	127	LYS	13
2	B	152	ASP	13
2	B	134	GLU	13
2	B	163	LYS	10
1	A	24	GLU	9
2	B	129	LYS	9
2	B	132	ASP	9
1	A	28	LEU	9
1	A	13	THR	8
1	A	30	ARG	8
1	A	17	GLN	7
2	B	113	ILE	6
2	B	107	THR	6
2	B	162	GLN	6
2	B	124	GLU	4
2	B	139	ASP	4
2	B	101	MET	4
2	B	111	LYS	3
2	B	149	GLN	3
1	A	10	GLN	3
1	A	15	MET	2
1	A	31	THR	2
2	B	165	SER	2
2	B	140	GLN	2
2	B	102	GLN	2
2	B	167	LEU	1
1	A	16	ASN	1
2	B	141	GLN	1
2	B	168	HIS	1
2	B	122	THR	1
2	B	148	LYS	1
2	B	157	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	12	CYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided