# W O R L D W I D E

# wwPDB

## P R O T E I N   D A T A   B A N K

# Full wwPDB NMR Structure Validation Report (i)

May 31, 2020 – 12:15 pm BST

| | | |
|---|---|---|
| PDB ID | : | 6RH6 |
| Title | : | Solution structure and 1H, 13C and 15N chemical shift assignments for the complex of NECAP1 PHear domain with phosphorylated AP2 mu2 148-163 |
| Authors | : | Owen, D.J.; Neuhaus, D.; Yang, J.-C.; Herrmann, T. |
| Deposited on | : | 2019-04-18 |

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

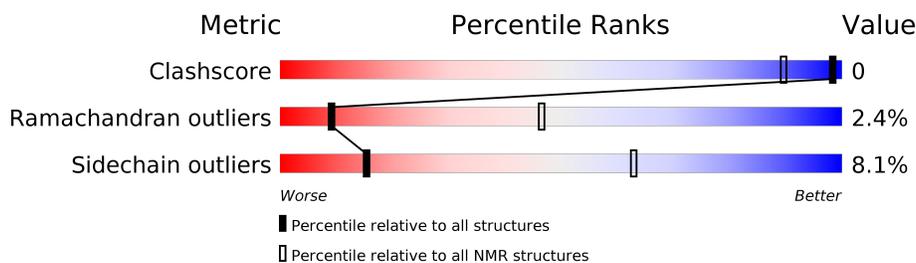| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance (i)

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 | Percentile Ranks | Value |
|---|---|---|
| Clashscore | | 0 |
| Ramachandran outliers | | 2.4% |
| Sidechain outliers | | 8.1% |

*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 | 138 | 71%    9% ••    18% |
| 2 | B | 15 | 100% |

# 2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 27 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:8-A:24, A:30-A:97, A:103-A:130 (113) | 0.21 | 27 |

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 7 clusters and 3 single-model clusters were found.

| Cluster number | Models |
|---|---|
| 1 | 2, 6, 16, 20, 21, 27, 29, 30 |
| 2 | 4, 7, 9, 11, 22 |
| 3 | 10, 18, 23, 24 |
| 4 | 13, 15, 17, 28 |
| 5 | 1, 19 |
| 6 | 5, 14 |
| 7 | 3, 8 |
| Single-model clusters | 12; 25; 26 |

# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2415 atoms, of which 1191 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adaptin ear-binding coat-associated protein 1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| | | | Total | C | H | N | O | S | |
| 1 | A | 138 | 2168 | 695 | 1069 | 190 | 212 | 2 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

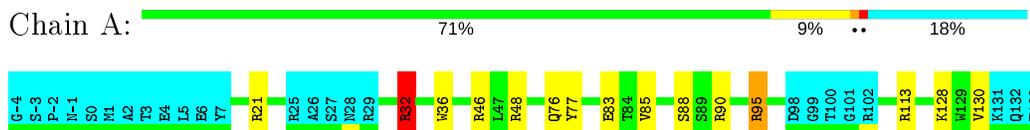| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | -4 | GLY | - | expression tag | UNP Q8NC96 |
| A | -3 | SER | - | expression tag | UNP Q8NC96 |
| A | -2 | PRO | - | expression tag | UNP Q8NC96 |
| A | -1 | ASN | - | expression tag | UNP Q8NC96 |
| A | 0 | SER | - | expression tag | UNP Q8NC96 |

- Molecule 2 is a protein called AP-2 complex subunit mu.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| | | | Total | C | H | N | O | P | |
| 2 | B | 15 | 247 | 73 | 122 | 25 | 26 | 1 | 0 |

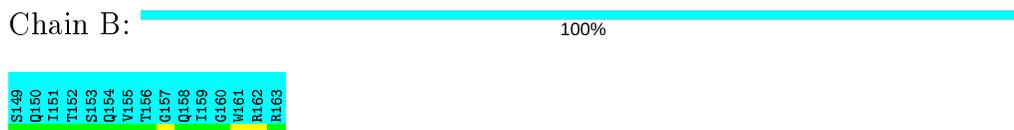# 4 Residue-property plots (i)

## 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: Adaptin ear-binding coat-associated protein 1

Chain A:

71%     9%   ••   18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R46 L47 R48 Q76 Y77 E83 T84 V85 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

- Molecule 2: AP-2 complex subunit mu

Chain B:

100%

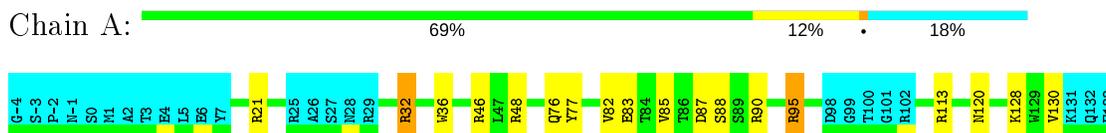S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

## 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

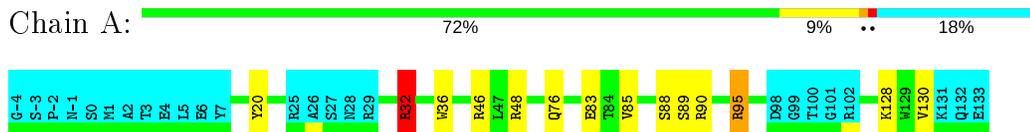- Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:

69%     12%   •   18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R46 L47 R48 Q76 Y77 V82 E83 T84 V85 T86 D87 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 N120 K128 W129 V130 K131 Q132 E133

- Molecule 2: AP-2 complex subunit mu

Chain B:

100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

### 4.2.2 Score per residue for model 2

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:

72%                                    9%  ··      18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 Y20 R25 A26 S27 N28 R29 R32 W36 R46 I47 R48 Q76 E83 T84 V85 S88 S89 R90 R95 D98 G99 T100 G101 R102 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:

100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

### 4.2.3 Score per residue for model 3

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:

71%                                    9%  ··      18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 D62 Q76 Y77 E83 T84 V85 S88 S89 R95 D98 G99 T100 G101 R102 R113 N120 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:

100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
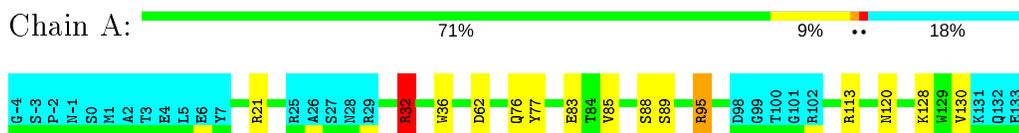
### 4.2.4 Score per residue for model 4

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:

72%                                    9%  ·       18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 R46 L47 R48 Q71 Q76 Y77 V82 E83 T84 V85 D98 G99 T100 G101 R102 R113 L123 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:

100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

### 4.2.5 Score per residue for model 5

• Molecule 1: Adaptin ear-binding coat-associated protein 1



• Molecule 2: AP-2 complex subunit mu



### 4.2.6 Score per residue for model 6

• Molecule 1: Adaptin ear-binding coat-associated protein 1
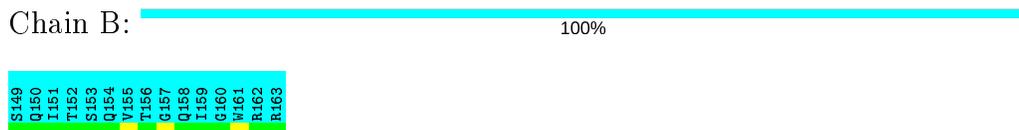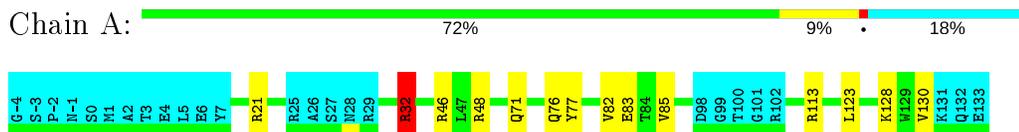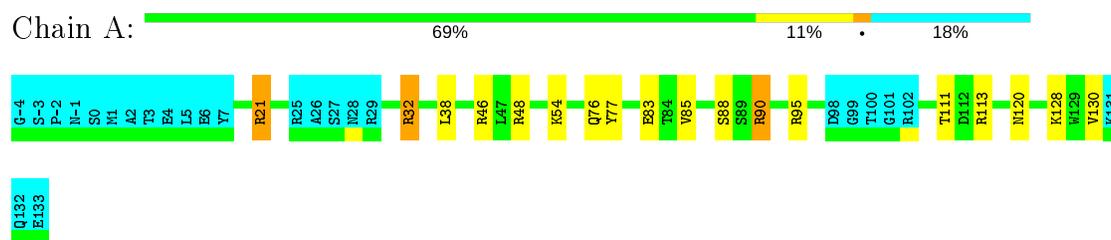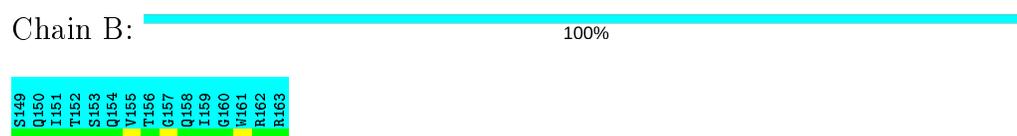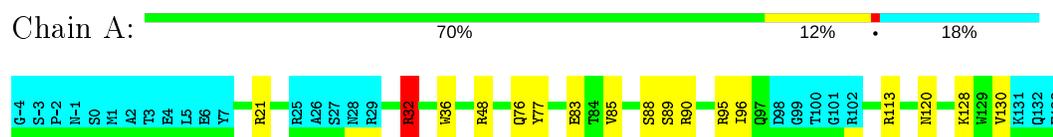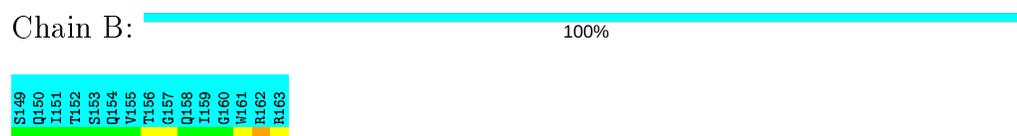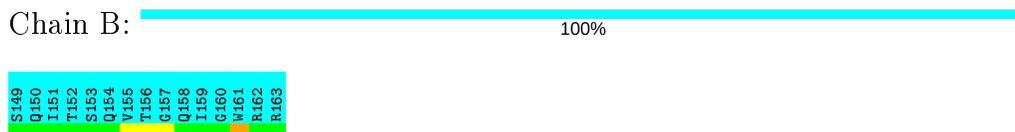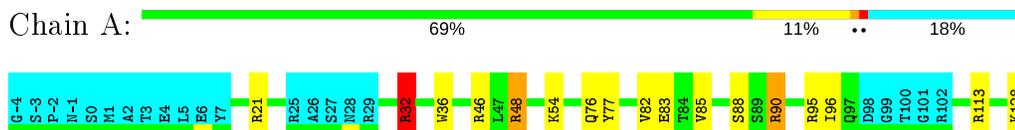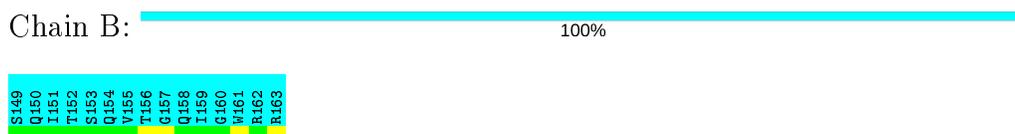


• Molecule 2: AP-2 complex subunit mu



### 4.2.7 Score per residue for model 7

• Molecule 1: Adaptin ear-binding coat-associated protein 1



• Molecule 2: AP-2 complex subunit mu

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

## 4.2.8 Score per residue for model 8

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 69% 12% •• 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 G30 Y31 R32 W36 R46 L47 R48 K54 D62 Q76 Y77 V82 E83 T84 V85 R95 D98 G99 T100 G101 R102 R113 L123 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

## 4.2.9 Score per residue for model 9

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 72% 8% •• 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 Y20 R25 A26 S27 N28 R29 R32 W36 R48 Q76 Y77 E83 T84 V85 S88 R95 D98 G99 T100 G101 R102 R113 N120 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

## 4.2.10 Score per residue for model 10

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 71% 9% • 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 E8 R21 R25 A26 S27 N28 R29 R32 R46 L47 R48 K54 Q76 E83 T84 V85 T86 D87 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

### 4.2.11 Score per residue for model 11

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 69% 11% •• 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R46 L47 R48 K54 Q76 Y77 V82 E83 T84 V85 S88 S89 R90 R95 I96 Q97 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163

### 4.2.12 Score per residue for model 12

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 71% 9% • 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 V13 R25 A26 S27 N28 R29 R32 R46 L47 R48 Q76 Y77 V82 E83 T84 V85 R95 I96 Q97 D98 G99 T100 G101 R102 L123 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
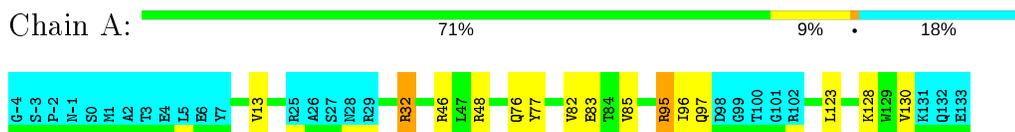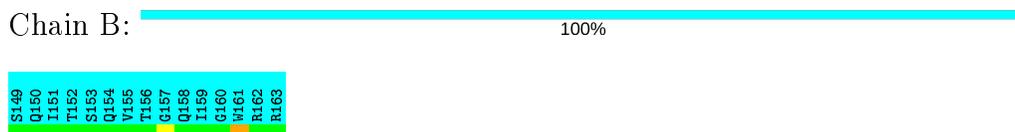
### 4.2.13 Score per residue for model 13

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 72% 9% • 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 R48 Q76 Y77 V82 E83 T84 V85 S89 R90 R95 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
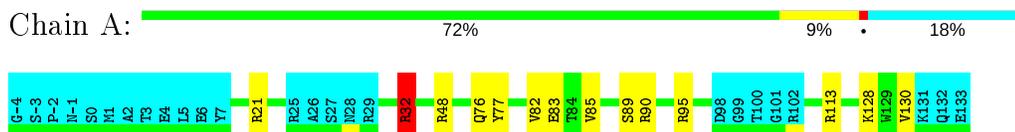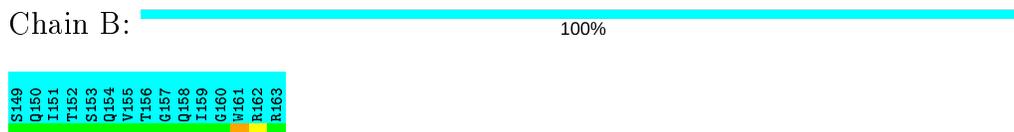
### 4.2.14 Score per residue for model 14

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 71% 7% • 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R48 Q76 Y77 E83 T84 V85 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 N120 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
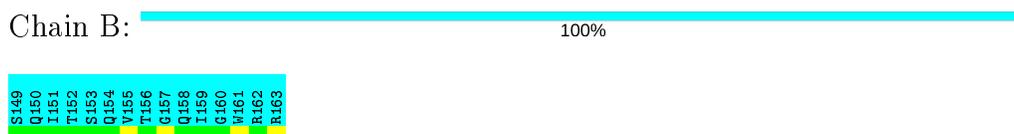
### 4.2.15 Score per residue for model 15

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 70% 10% •• 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 E8 R21 R25 A26 S27 N28 R29 G30 Y31 R32 R46 L47 R48 T55 V74 E75 Q76 Y77 E83 T84 V85 R95 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
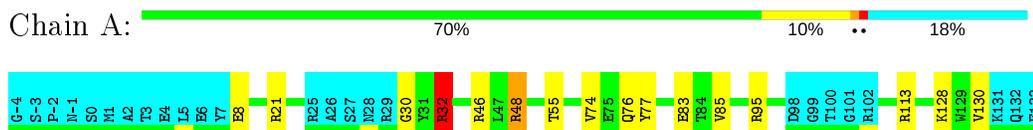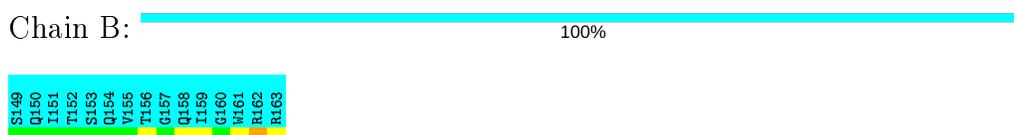
### 4.2.16 Score per residue for model 16

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 71% 9% •• 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 A33 S34 Q76 Y77 E83 T84 V85 S88 S89 R95 I96 Q97 D98 G99 T100 G101 R102 T111 D112 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
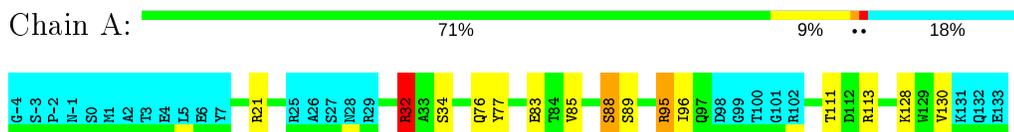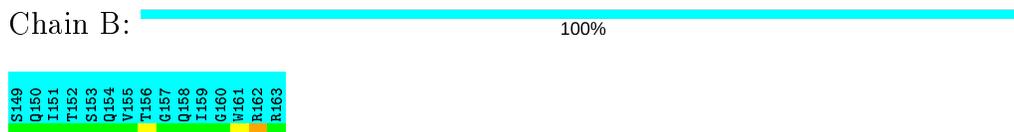
## 4.2.17 Score per residue for model 17

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 72% 8% •• 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 R46 L47 R48 Q76 Y77 V82 E83 T84 V85 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 K128 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
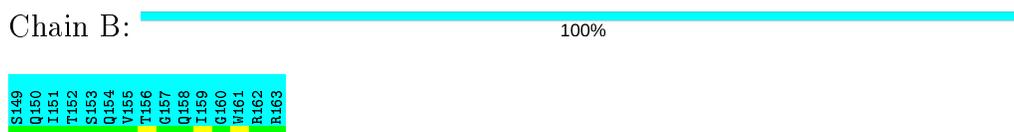
## 4.2.18 Score per residue for model 18

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 73% 8% • 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R25 A26 S27 N28 R29 R32 W36 K37 L38 R46 L47 R48 Q76 E83 T84 V85 S88 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
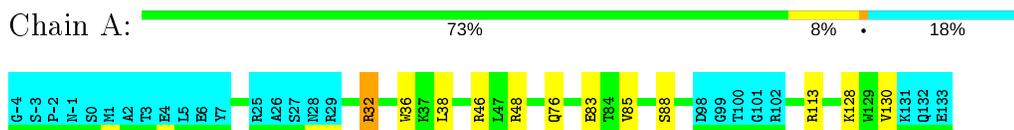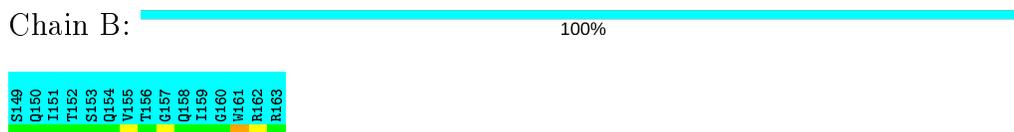
## 4.2.19 Score per residue for model 19

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 72% 8% •• 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 R46 L47 R48 Q76 Y77 E83 T84 V85 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:                                              100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
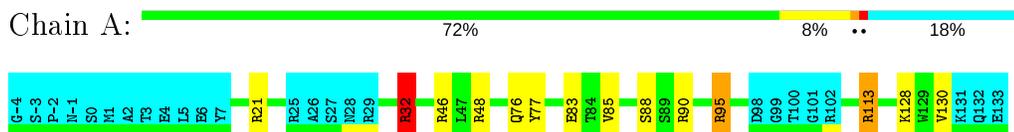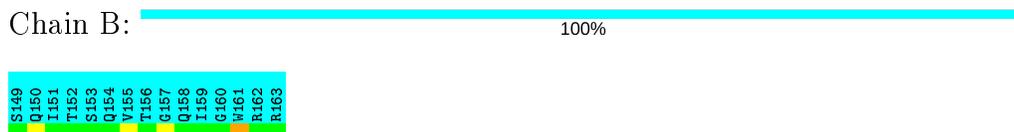
### 4.2.20 Score per residue for model 20

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:                          73%                          7%  ••       18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R48 Q76 Y77 E83 T84 V85 R95 D98 G99 T100 G101 R102 R113 N120 K128 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:                                              100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
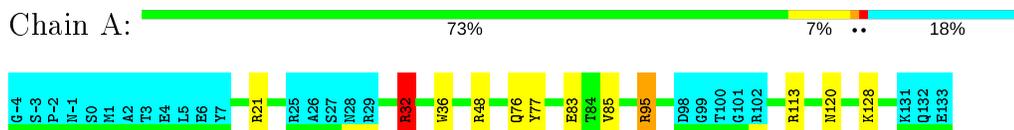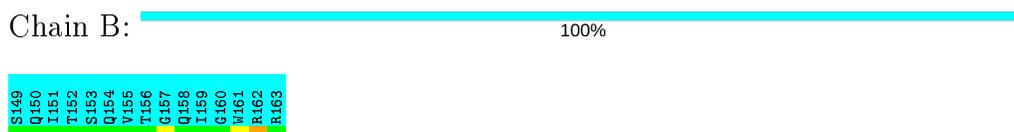
### 4.2.21 Score per residue for model 21

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:                          72%                          7%  ••       18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 Q76 Y77 E83 T84 V85 R90 R95 D98 G99 T100 G101 R102 R113 N120 V121 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:                                              100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
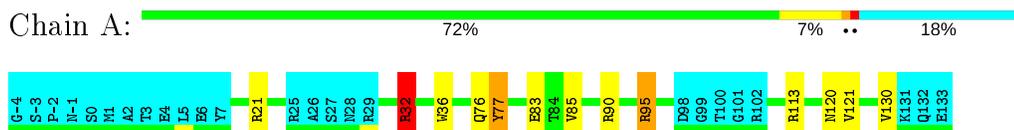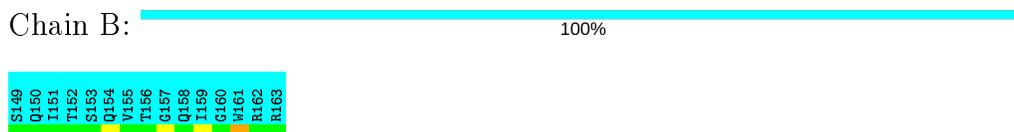
### 4.2.22 Score per residue for model 22

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:                          70%                          10%  ••       18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R25 A26 S27 N28 R29 R32 W36 K37 L38 R46 L47 R48 K54 Q76 Y77 E83 T84 V85 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:	100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
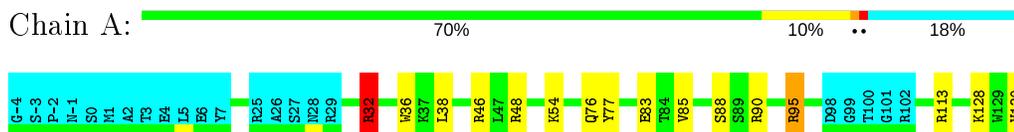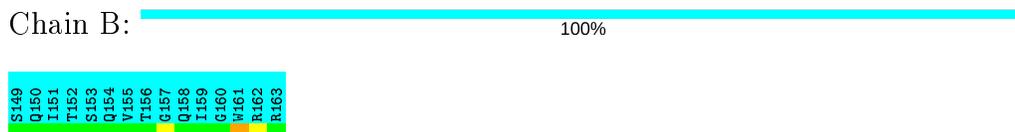
### 4.2.23 Score per residue for model 23

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:	73%	7%	..	18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 R46 L47 R48 K54 Q76 E83 T84 V85 R95 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:	100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
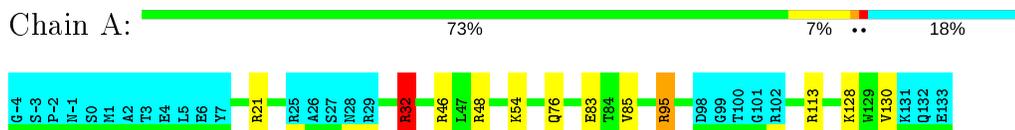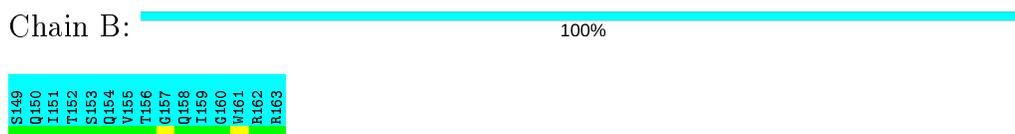
### 4.2.24 Score per residue for model 24

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:	73%	7%	·	18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R25 A26 S27 N28 R29 R32 W36 R46 K54 T55 Q76 E83 T84 V85 R95 D98 G99 T100 G101 R102 R113 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:	100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
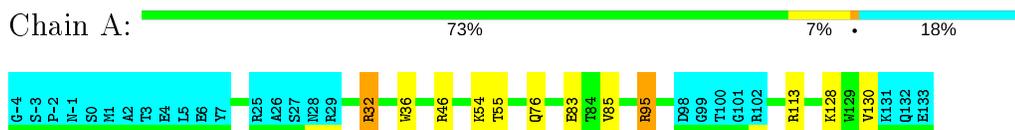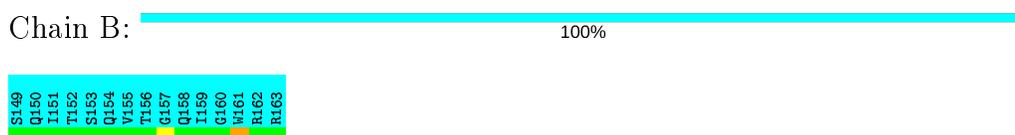
### 4.2.25 Score per residue for model 25

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:	72%	9%	··	18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R46 L47 R48 K54 Q76 E83 T84 V85 S88 S89 R90 R95 D98 G99 T100 G101 R102 R113 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:      100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
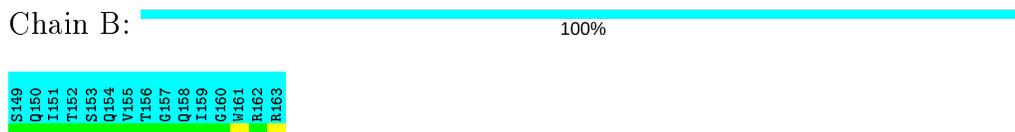
### 4.2.26    Score per residue for model 26

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:      72%      8%  ••   18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 K54 Q76 Y77 E83 T84 V85 R95 I96 Q97 D98 G99 T100 G101 R102 N120 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:      100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
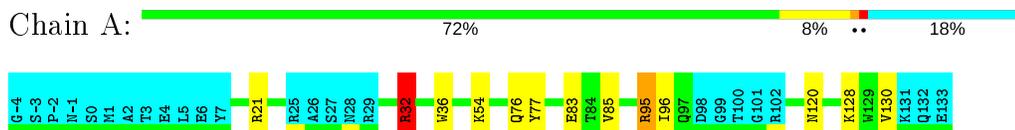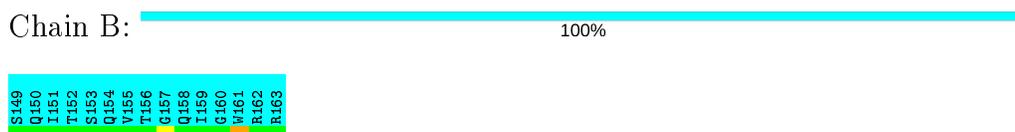
### 4.2.27    Score per residue for model 27 (medoid)

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:      74%      7%  ••   18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 E8 R25 A26 S27 N28 R29 R32 R46 L47 R48 Q76 E83 T84 V85 R90 R95 D98 G99 T100 G101 R102 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B:      100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
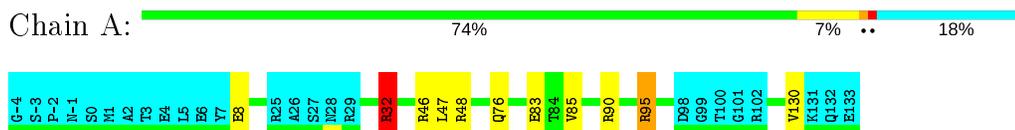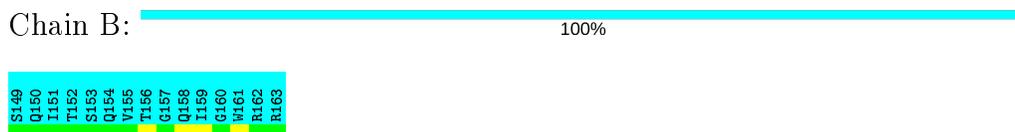
### 4.2.28    Score per residue for model 28

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A:      70%      10%  ••   18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 R46 L47 R48 T55 V64 Q76 Y77 V82 E83 T84 V85 R95 D98 G99 T100 G101 R102 T111 D112 R113 N120 K128 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
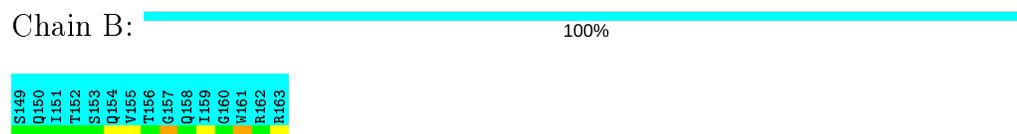
### 4.2.29 Score per residue for model 29

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 72% 9% · 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R46 I47 R48 Q76 Y77 E83 T84 V85 S88 S89 I96 Q97 D98 G99 T100 G101 R102 N120 K128 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
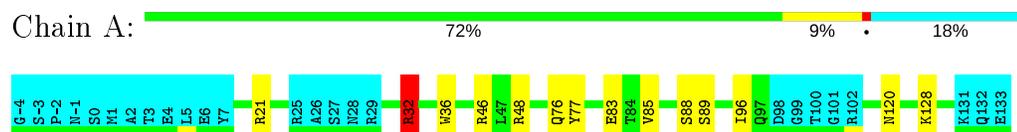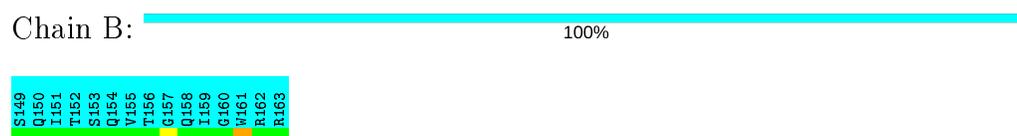
### 4.2.30 Score per residue for model 30

• Molecule 1: Adaptin ear-binding coat-associated protein 1

Chain A: 72% 8% · 18%

G-4 S-3 P-2 N-1 S0 M1 A2 T3 E4 L5 E6 Y7 R21 R25 A26 S27 N28 R29 R32 W36 R48 Q76 Y77 E83 T84 V85 R95 I96 Q97 D98 G99 T100 G101 R102 N120 K128 W129 V130 K131 Q132 E133

• Molecule 2: AP-2 complex subunit mu

Chain B: 100%

S149 Q150 I151 T152 S153 Q154 V155 T156 G157 Q158 I159 G160 W161 R162 R163
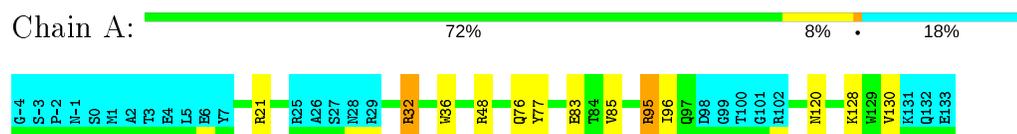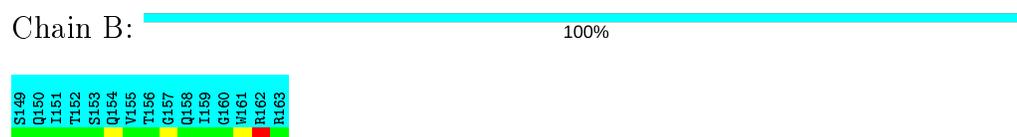
# 5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 30 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 |
|---|---|---|
| UNIO | structure calculation | 2.8.1 |
| Xplor-NIH | structure calculation | 2.28 |
| Amber | structure calculation | 11 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

| Chemical shift file(s) | input_cs.cif |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 1655 |
| Number of shifts mapped to atoms | 1655 |
| 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.

COVALENT-GEOMETRY INFOmissingINFO

## 5.1 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 | 907 | 889 | 889 | 0±1 |
| 2 | B | 0 | 0 | 0 | 0±0 |
| All | All | 27210 | 26670 | 26670 | 12 |

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 0.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|--------|--------|----------|-------------|--------|--------|
| | | | | Worst | Total |
| 1:A:77:TYR:CD2 | 1:A:82:VAL:HG13 | 0.66 | 2.26 | 4 | 2 |
| 1:A:77:TYR:CD1 | 1:A:82:VAL:HG13 | 0.64 | 2.27 | 12 | 6 |
| 1:A:82:VAL:HG11 | 1:A:123:LEU:HD13 | 0.56 | 1.78 | 4 | 3 |
| 1:A:38:LEU:HD23 | 1:A:38:LEU:H | 0.41 | 1.76 | 22 | 1 |

## 5.2 Torsion angles (i)

### 5.2.1 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 | 113/138 (82%) | 100±2 (89±2%) | 10±2 (9±2%) | 3±1 (2±1%) | 9 | 46 |
| 2 | B | 0 | - | - | - | - | |
| All | All | 3390/4590 (74%) | 3002 (89%) | 308 (9%) | 80 (2%) | 9 | 46 |

All 7 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 | 32 | ARG | 30 |
| 1 | A | 85 | VAL | 30 |
| 1 | A | 21 | ARG | 9 |
| 1 | A | 54 | LYS | 8 |
| 1 | A | 30 | GLY | 1 |
| 1 | A | 13 | VAL | 1 |
| 1 | A | 34 | SER | 1 |

### 5.2.2 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 | 98/118 (83%) | 90±1 (92±1%) | 8±1 (8±1%) | 15 | 63 |
| 2 | B | 0 | - | - | - | |
| All | All | 2940/3900 (75%) | 2703 (92%) | 237 (8%) | 15 | 63 |

All 26 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 | 32 | ARG | 30 |
| 1 | A | 76 | GLN | 30 |
| 1 | A | 83 | GLU | 30 |
| 1 | A | 130 | VAL | 26 |
| 1 | A | 128 | LYS | 25 |
| 1 | A | 95 | ARG | 24 |
| 1 | A | 36 | TRP | 17 |
| 1 | A | 120 | ASN | 13 |
| 1 | A | 113 | ARG | 7 |
| 1 | A | 88 | SER | 6 |
| 1 | A | 55 | THR | 3 |
| 1 | A | 48 | ARG | 3 |
| 1 | A | 111 | THR | 3 |
| 1 | A | 8 | GLU | 3 |
| 1 | A | 87 | ASP | 2 |
| 1 | A | 84 | THR | 2 |
| 1 | A | 38 | LEU | 2 |
| 1 | A | 20 | TYR | 2 |
| 1 | A | 62 | ASP | 2 |
| 1 | A | 54 | LYS | 1 |
| 1 | A | 64 | VAL | 1 |
| 1 | A | 71 | GLN | 1 |
| 1 | A | 121 | VAL | 1 |
| 1 | A | 90 | ARG | 1 |
| 1 | A | 97 | GLN | 1 |
| 1 | A | 74 | VAL | 1 |

### 5.2.3   RNA (i)

There are no RNA molecules in this entry.

## 5.3   Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------|------|-------|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | TPO | B | 156 | 2 | 8,10,11 | 1.08±0.04 | 0±0 (0±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|--------|------|-------|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | TPO | B | 156 | 2 | 10,14,16 | 1.13±0.15 | 0±0 (0±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 2 | TPO | B | 156 | 2 | - | 0±0,9,11,13 | - |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique torsion outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|-------|----------------|
| 2 | B | 156 | TPO | N-CA-CB-OG1 | 4 |

There are no ring outliers.

## 5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.5 Ligand geometry (i)

There are no ligands in this entry.

## 5.6 Other polymers (i)

There are no such molecules in this entry.

## 5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 77% for the entire structure.

## 6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *starch_output*

### 6.1.1 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 | 1655 |
| Number of shifts mapped to atoms | 1655 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 4 |

### 6.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 138 | 0.03 ± 0.13 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 121 | -0.22 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 0 | — | None (insufficient data) |
| $^{15}N$ | 127 | 0.33 ± 0.38 | None needed (< 0.5 ppm) |

### 6.1.3 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. 1167 atoms were assigned a chemical shift out of a possible 1410. 17 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^1$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 436/553 (79%) | 218/220 (99%) | 113/226 (50%) | 105/107 (98%) |
| Sidechain | 591/711 (83%) | 367/417 (88%) | 217/260 (83%) | 7/34 (21%) |

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|  | **Total** | **$^1$H** | **$^{13}$C** | **$^{15}$N** |
|---|---|---|---|---|
| Aromatic | 140/146 (96%) | 73/77 (95%) | 64/65 (98%) | 3/4 (75%) |
| Overall | 1167/1410 (83%) | 658/714 (92%) | 394/551 (72%) | 115/145 (79%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1461 atoms were assigned a chemical shift out of a possible 1892. 18 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|  | **Total** | **$^1$H** | **$^{13}$C** | **$^{15}$N** |
|---|---|---|---|---|
| Backbone | 555/746 (74%) | 290/297 (98%) | 138/304 (45%) | 127/145 (88%) |
| Sidechain | 752/980 (77%) | 487/577 (84%) | 255/347 (73%) | 10/56 (18%) |
| Aromatic | 154/166 (93%) | 83/87 (95%) | 68/74 (92%) | 3/5 (60%) |
| Overall | 1461/1892 (77%) | 860/961 (89%) | 461/725 (64%) | 140/206 (68%) |

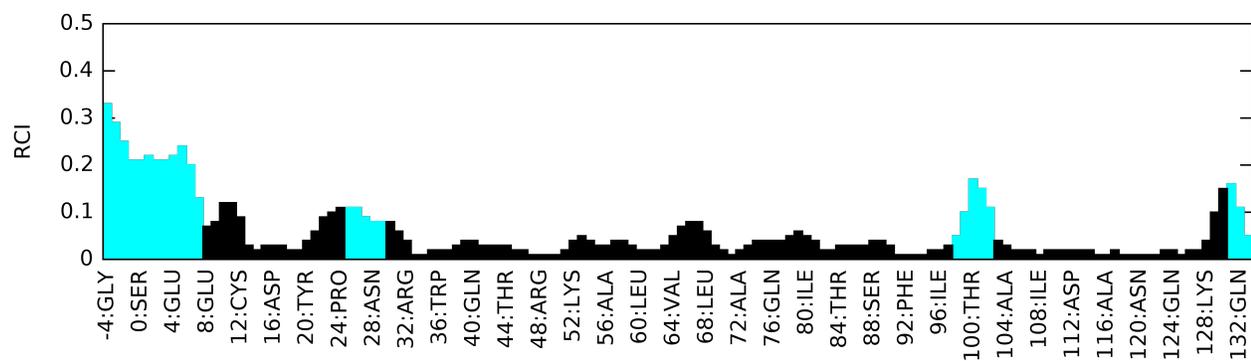### 6.1.4 Statistically unusual chemical shifts (i)

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

| **Mol** | **Chain** | **Res** | **Type** | **Atom** | **Shift, *ppm*** | **Expected range, *ppm*** | **Z-score** |
|---|---|---|---|---|---|---|---|
| 1 | A | 33 | ALA | HA | 1.46 | 6.46 − 2.06 | -6.4 |
| 1 | A | 33 | ALA | HB1 | -0.13 | 2.61 − 0.11 | -5.9 |
| 1 | A | 33 | ALA | HB3 | -0.13 | 2.61 − 0.11 | -5.9 |
| 1 | A | 33 | ALA | HB2 | -0.13 | 2.61 − 0.11 | -5.9 |

### 6.1.5 Random Coil Index (RCI) plots (i)

The images below report *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:

Random coil index (RCI) for chain B: