# Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 04:46 PM EST

| | | |
|---|---|---|
| PDB ID | : | 1CNP |
| Title | : | THE STRUCTURE OF CALCYCLIN REVEALS A NOVEL HOMODIMERIC FOLD FOR S100 CA2+-BINDING PROTEINS, NMR, 22 STRUCTURES |
| Authors | : | Potts, B.C.M.; Smith, J.; Akke, M.; Macke, T.J.; Okazaki, K.; Hidaka, H.; Case, D.A.; Chazin, W.J. |
| Deposited on | : | 1995-08-31 |

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

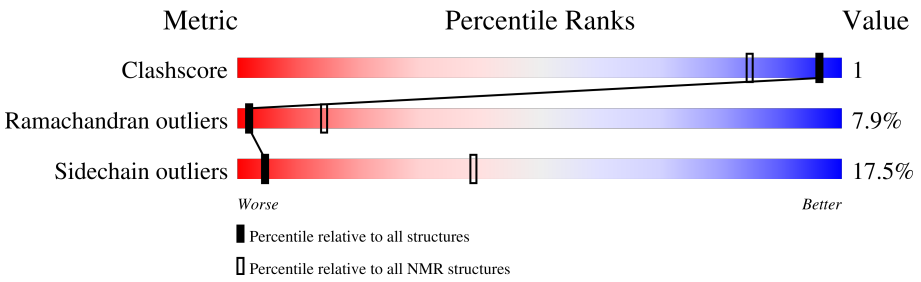
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.26 |
| Ideal geometry (proteins) | :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

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 90 | 49% 20% 31% |
| 1 | B | 90 | 56% 13% • 30% |

# 2 Ensemble composition and analysis (i)

This entry contains 22 models. Model 17 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:9-A:20, A:26-A:44, A:56-A:86, B:8-B:21, B:26-B:45, B:58-B:86 (125) | 1.37 | 17 |

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 and 3 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2896 atoms, of which 1470 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALCYCLIN (RABBIT, APO).

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 90 | 1448 | 455 | 735 | 116 | 139 | 3 | 0 |
| 1 | B | 90 | 1448 | 455 | 735 | 116 | 139 | 3 | 0 |

# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

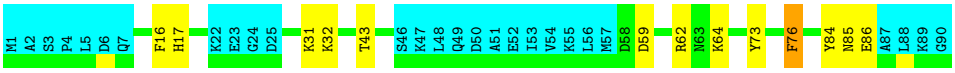
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 49% 20% 31%

• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B: 56% 13% • 30%



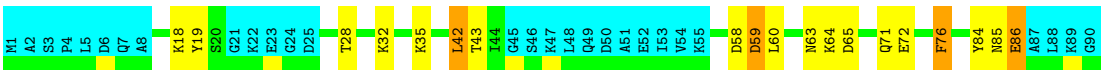

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

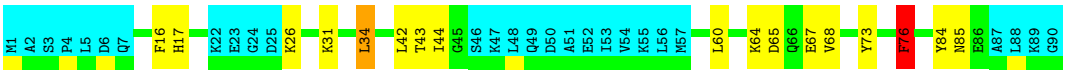
• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 48% 17% • 31%




• Molecule 1: CALCYCLIN (RABBIT, APO)

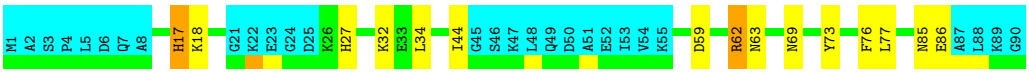
Chain B: 51% 17% •• 30%




### 4.2.2 Score per residue for model 2

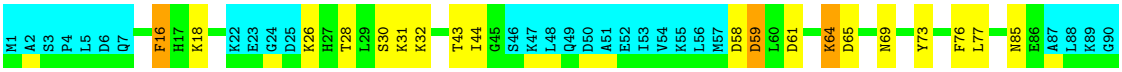
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A:




- Molecule 1: CALCYCLIN (RABBIT, APO)

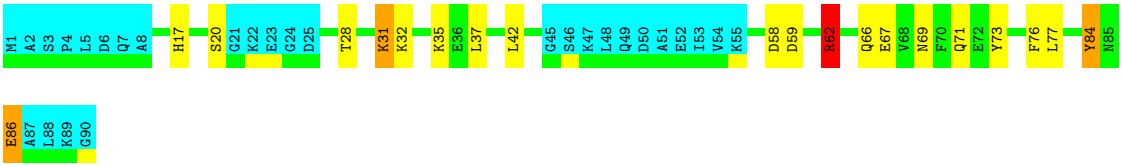
Chain B:




### 4.2.3 Score per residue for model 3

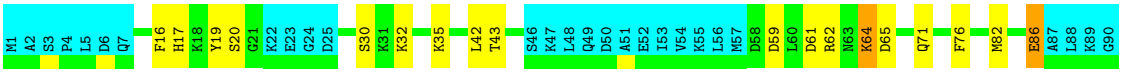
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A:




- Molecule 1: CALCYCLIN (RABBIT, APO)

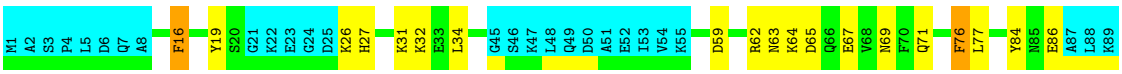
Chain B:

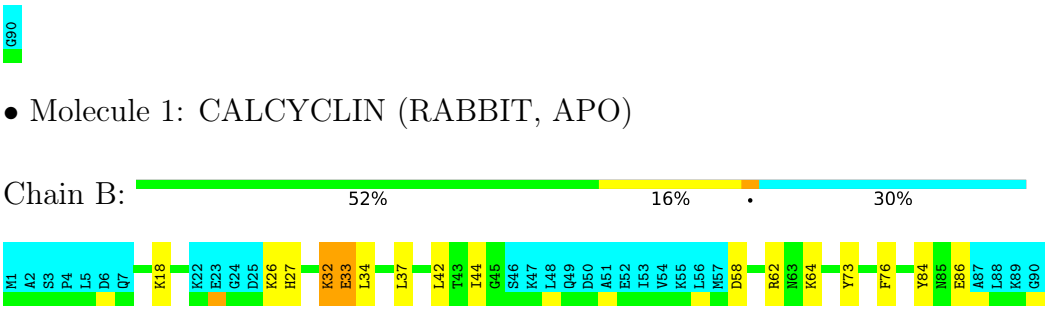



### 4.2.4 Score per residue for model 4

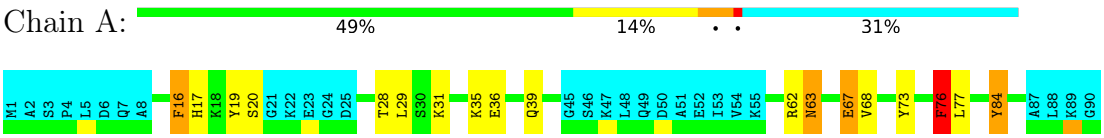
- Molecule 1: CALCYCLIN (RABBIT, APO)

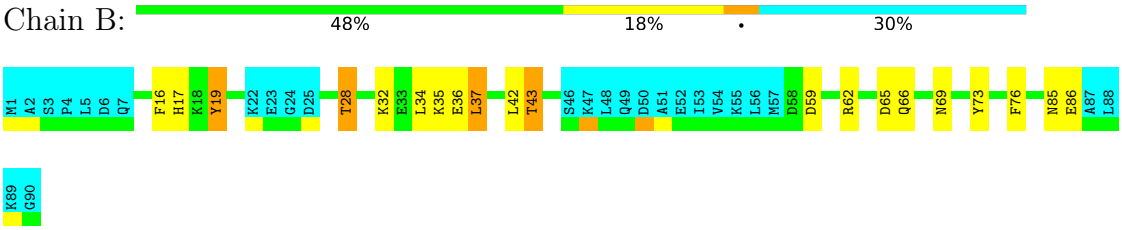
Chain A:



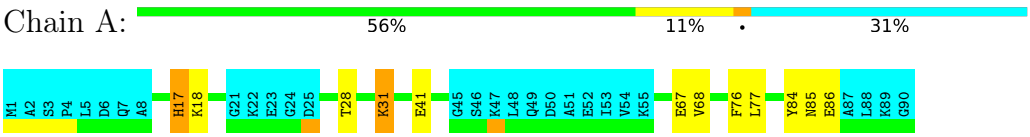


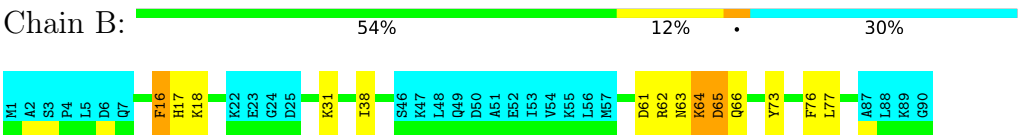

### 4.2.5 Score per residue for model 5




### 4.2.6 Score per residue for model 6

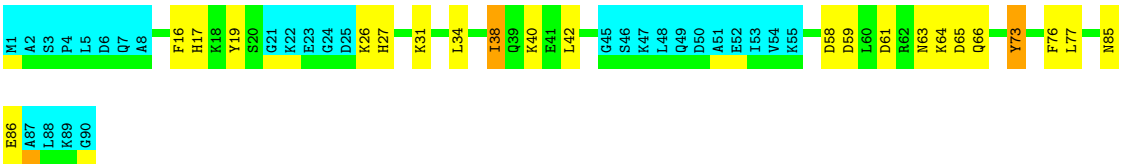


### 4.2.7 Score per residue for model 7

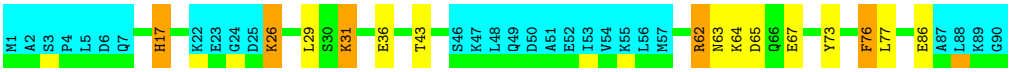
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 44% 22% • 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

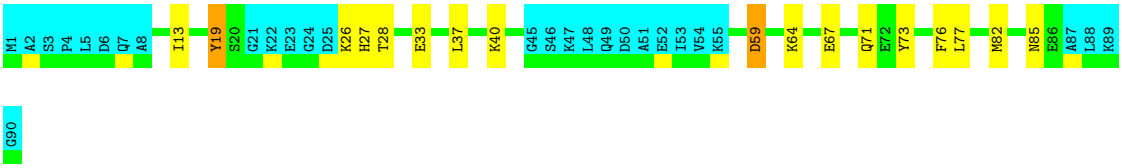
Chain B: 53% 11% 6% 30%




### 4.2.8 Score per residue for model 8

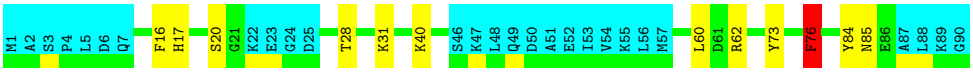
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 50% 17% • 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

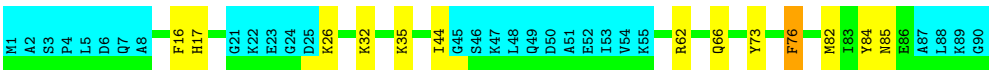
Chain B: 57% 12% • 30%




### 4.2.9 Score per residue for model 9

- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 54% 13% • 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B: 53% 14% • 30%

M1 A2 S3 P4 L5 D6 Q7 F16 H17 K18 Y19 K22 E23 G24 D25 K26 E36 E41 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 L56 M57 D58 D59 R62 N63 K64 D65 Y73 F76 Y84 N85 E86 A87 L88 K89 G90

### 4.2.10 Score per residue for model 10

- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 54% 13% • 31%

M1 A2 S3 P4 L5 D6 Q7 A8 L11 H17 K18 Y19 S20 G21 K22 E23 G24 D25 K31 K32 L42 T43 I44 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 R62 N63 Q71 E72 Y73 F76 Y84 A87 L88 K89 G90

- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B: 54% 12% • 30%

M1 A2 S3 P4 L5 D6 Q7 I13 F16 H17 K18 K22 E23 G24 D25 K32 K35 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 L56 M57 D58 D59 R62 Q66 N69 F70 Y73 F76 Y84 A87 L88 K89 G90

### 4.2.11 Score per residue for model 11

- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 53% 14% • 31%

M1 A2 S3 P4 L5 D6 Q7 A8 F16 H17 G21 K22 E23 G24 D25 K26 H27 I38 Q39 K40 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 D58 D59 L60 D61 D65 N69 F70 Q71 F76 L77 Y84 A87 L88 K89 G90

- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B: 49% 18% • 30%

M1 A2 S3 P4 L5 D6 Q7 H17 K18 Y19 K22 E23 G24 D25 K26 H27 L34 L37 E41 L42 T43 I44 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 L56 M57 N63 K64 D65 Q66 Q71 E72 Y73 F76 L77 N85 E86 A87 L88 K89 G90

### 4.2.12 Score per residue for model 12

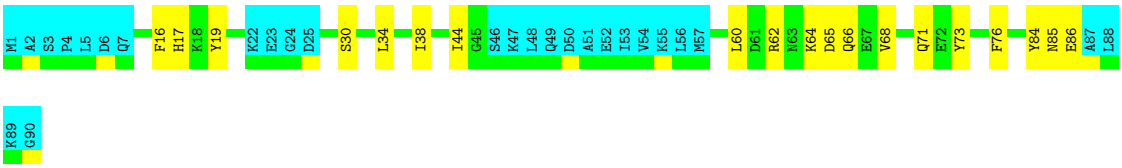
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 49% 16% • 31%

M1 A2 S3 P4 L5 D6 Q7 A8 H17 K18 Y19 S20 G21 K22 E23 G24 D25 T28 K32 I38 Q39 K40 E41 L42 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 D59 L60 D61 R62 E72 Y73 I74 T75 F76 Y84 N85 E86 A87 L88 K89 G90

- Molecule 1: CALCYCLIN (RABBIT, APO)

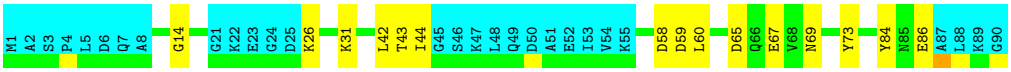
Chain B: 49% 21% 30%




### 4.2.13 Score per residue for model 13

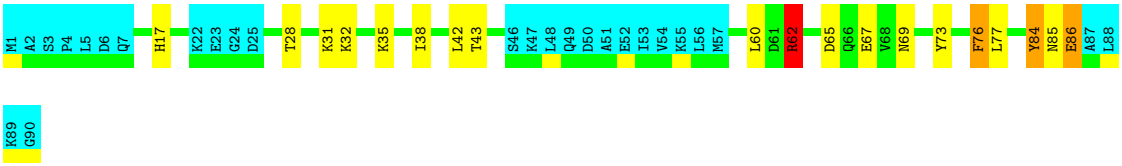
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 52% 17% 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

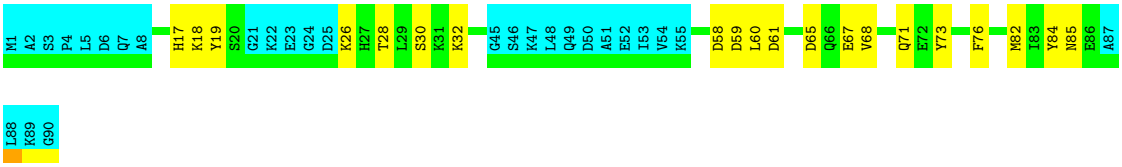
Chain B: 49% 17% • • 30%




### 4.2.14 Score per residue for model 14

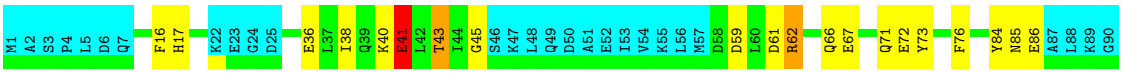
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 47% 22% 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

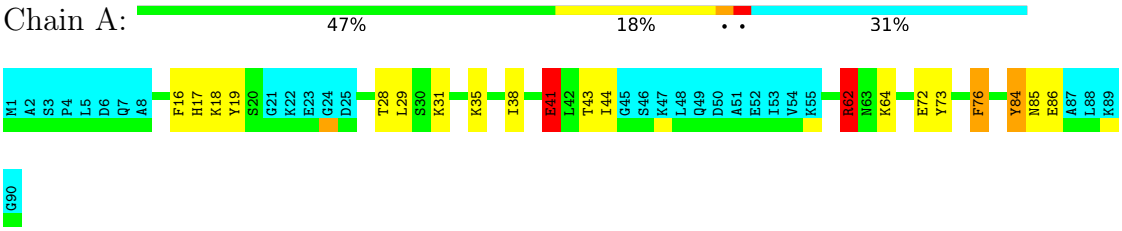
Chain B: 48% 19% • • 30%



### 4.2.15 Score per residue for model 15

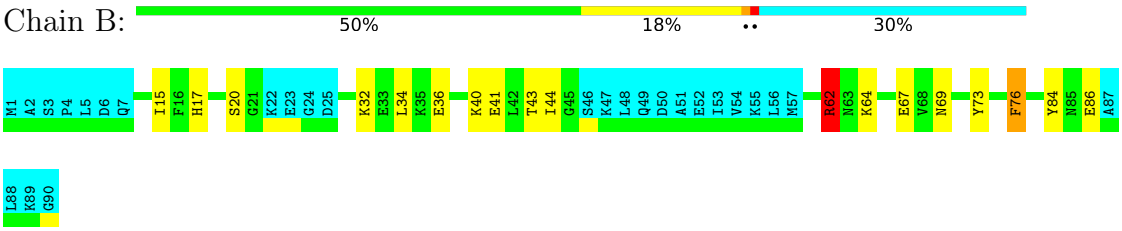
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A:




- Molecule 1: CALCYCLIN (RABBIT, APO)

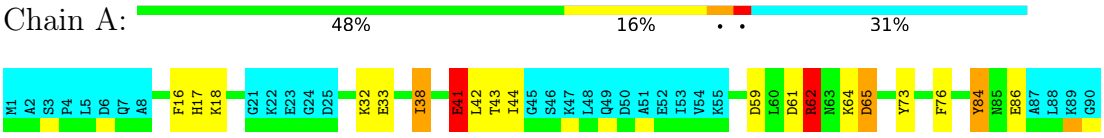
Chain B:




### 4.2.16 Score per residue for model 16

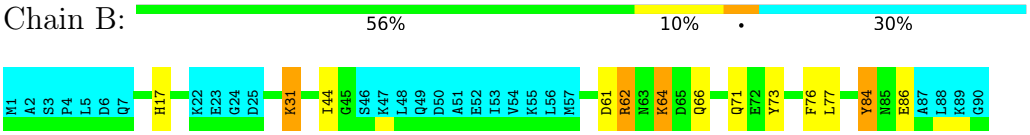
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A:




- Molecule 1: CALCYCLIN (RABBIT, APO)

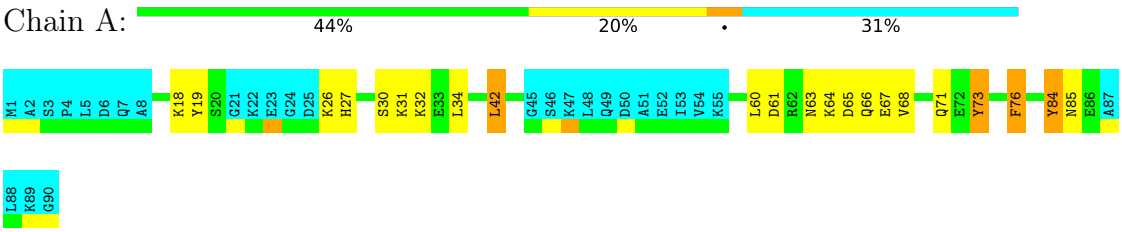
Chain B:




### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A:



• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B: 41% 22% 6% • 30%

M1 A2 S3 P4 L5 D6 Q7 L11 F16 H17 K18 Y19 S20 G21 K22 E23 G24 D25 K26 H27 T28 L29 S30 K31 K32 K35 L42 T43 I44 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 L56 M57 D58 D59 L60 D61 R62 N63 K64 D65 Q66 F76 I83 Y84 N85 E86 A87 L88 K89 G90

### 4.2.18 Score per residue for model 18

• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 50% 14% • • 31%

M1 A2 S3 P4 L5 D6 Q7 A8 F16 H17 K18 G21 K22 E23 G24 D25 S30 K31 K35 E36 L37 I38 E41 L42 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 N63 K64 E67 Q71 F76 Y84 N85 E86 A87 L88 K89 G90

• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B: 54% 10% • • 30%

M1 A2 S3 P4 L5 D6 Q7 H17 K18 K22 E23 G24 D25 K35 I38 Q39 K40 E41 L42 T43 I44 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 L56 M57 D61 R62 N63 K64 F76 Y84 A87 L88 K89 G90

### 4.2.19 Score per residue for model 19

• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 52% 10% 6% • 31%

M1 A2 S3 P4 L5 D6 Q7 A8 F16 H17 G21 K22 E23 G24 D25 K26 H27 S30 Q39 L42 G45 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 D59 R62 N63 E67 V68 N69 Y73 F76 Y84 N85 E86 A87 L88 K89 G90

• Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B: 47% 19% • 30%

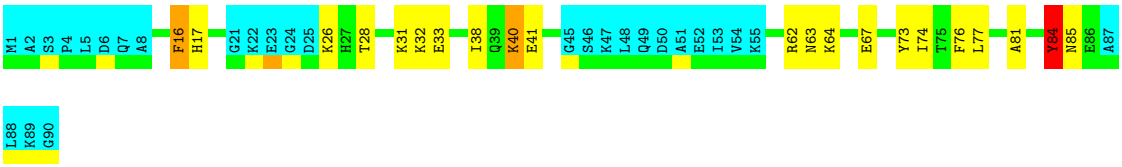
M1 A2 S3 P4 L5 D6 Q7 F16 H17 K18 Y19 K22 E23 G24 D25 K26 H27 T28 K31 L34 L37 L42 S46 K47 L48 Q49 D50 A51 E52 I53 V54 K55 L56 M57 D58 D59 L60 N63 K64 E72 Y73 F76 I83 Y84 N85 E86 A87 L88 K89

G90

### 4.2.20 Score per residue for model 20

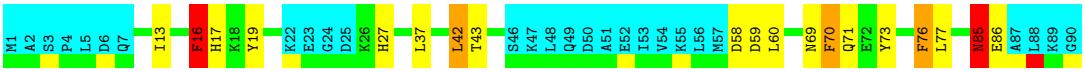
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 46% 20% • • 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

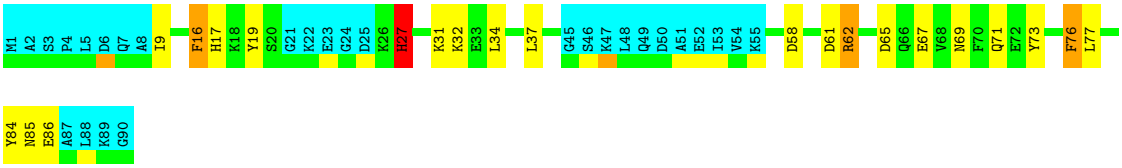
Chain B: 49% 16% • • 30%




### 4.2.21 Score per residue for model 21

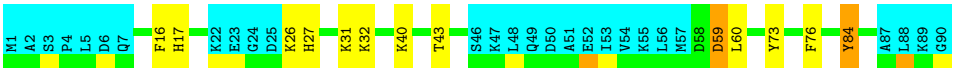
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 44% 20% • • 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

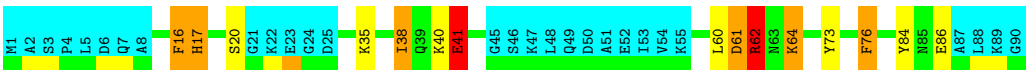
Chain B: 56% 12% • 30%




### 4.2.22 Score per residue for model 22

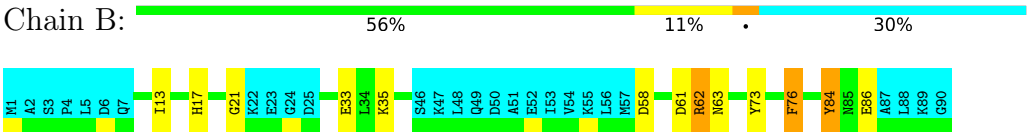
- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain A: 52% 8% 7% • 31%




- Molecule 1: CALCYCLIN (RABBIT, APO)

Chain B:


56%
11%
•
30%
M1
A2
S3
P4
L5
D6
Q7
I13
H17
G21
K22
E23
G24
D25
E33
L34
K35
S46
K47
L48
Q49
D50
A51
E52
I53
V54
K55
L56
M57
D58
D61
R62
N63
Y73
F76
Y84
N85
E86
A87
L88
K89
G90

# 5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 22 were deposited, based on the following criterion: *?*.

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

| Software name | Classification | Version |
|---|---|---|
| S | refinement | |

No chemical shift data was provided.

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.56±0.01 | 0±0/522 ( 0.0± 0.0%) | 1.00±0.05 | 1±1/700 ( 0.1± 0.2%) |
| 1 | B | 0.56±0.01 | 0±0/519 ( 0.0± 0.0%) | 1.00±0.05 | 1±1/696 ( 0.1± 0.1%) |
| All | All | 0.56 | 0/22902 ( 0.0%) | 1.00 | 36/30712 ( 0.1%) |

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

| Mol | Chain | Chirality | Planarity |
|---|---|---|---|
| 1 | A | 0.0±0.0 | 3.6±1.1 |
| 1 | B | 0.0±0.0 | 3.5±1.1 |
| All | All | 0 | 155 |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 62 | ARG | NE-CZ-NH1 | 8.82 | 124.71 | 120.30 | 15 | 2 |
| 1 | B | 76 | PHE | CB-CG-CD1 | -8.35 | 114.96 | 120.80 | 18 | 6 |
| 1 | A | 62 | ARG | NE-CZ-NH2 | -7.44 | 116.58 | 120.30 | 21 | 1 |
| 1 | B | 62 | ARG | NE-CZ-NH1 | 7.32 | 123.96 | 120.30 | 16 | 1 |
| 1 | B | 41 | GLU | N-CA-CB | -7.20 | 97.64 | 110.60 | 14 | 2 |
| 1 | B | 59 | ASP | C-N-CA | 7.13 | 139.52 | 121.70 | 21 | 2 |
| 1 | A | 76 | PHE | CB-CG-CD1 | -6.78 | 116.05 | 120.80 | 12 | 6 |
| 1 | A | 41 | GLU | N-CA-CB | -6.75 | 98.46 | 110.60 | 16 | 2 |
| 1 | A | 84 | TYR | CB-CG-CD2 | -6.48 | 117.11 | 121.00 | 20 | 1 |
| 1 | A | 61 | ASP | C-N-CA | 6.33 | 137.52 | 121.70 | 22 | 1 |
| 1 | A | 16 | PHE | CB-CG-CD1 | -6.20 | 116.46 | 120.80 | 20 | 1 |
| 1 | A | 76 | PHE | CB-CG-CD2 | -6.11 | 116.52 | 120.80 | 22 | 1 |
| 1 | A | 62 | ARG | CD-NE-CZ | 5.77 | 131.68 | 123.60 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 42 | LEU | CB-CA-C | 5.76 | 121.15 | 110.20 | 18 | 1 |
| 1 | B | 62 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 | 8 | 3 |
| 1 | A | 41 | GLU | N-CA-C | 5.60 | 126.12 | 111.00 | 22 | 1 |
| 1 | B | 84 | TYR | CB-CG-CD2 | -5.45 | 117.73 | 121.00 | 16 | 1 |
| 1 | A | 85 | ASN | N-CA-C | 5.30 | 125.31 | 111.00 | 19 | 1 |
| 1 | A | 16 | PHE | CB-CG-CD2 | -5.29 | 117.10 | 120.80 | 5 | 1 |
| 1 | A | 84 | TYR | CA-CB-CG | 5.06 | 123.01 | 113.40 | 3 | 1 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | A | 76 | PHE | Sidechain | 21 |
| 1 | B | 76 | PHE | Sidechain | 21 |
| 1 | B | 73 | TYR | Sidechain | 18 |
| 1 | A | 73 | TYR | Sidechain | 16 |
| 1 | A | 84 | TYR | Sidechain | 13 |
| 1 | A | 19 | TYR | Sidechain | 11 |
| 1 | B | 84 | TYR | Sidechain | 7 |
| 1 | A | 17 | HIS | Sidechain | 7 |
| 1 | B | 17 | HIS | Sidechain | 7 |
| 1 | B | 19 | TYR | Sidechain | 7 |
| 1 | B | 62 | ARG | Sidechain | 7 |
| 1 | B | 16 | PHE | Sidechain | 6 |
| 1 | A | 62 | ARG | Sidechain | 5 |
| 1 | A | 27 | HIS | Sidechain | 3 |
| 1 | A | 16 | PHE | Sidechain | 3 |
| 1 | B | 27 | HIS | Sidechain | 2 |
| 1 | B | 70 | PHE | Sidechain | 1 |

## 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 | 514 | 530 | 530 | 1±1 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | B | 511 | 521 | 521 | 1±1 |
| All | All | 22550 | 23122 | 23122 | 38 |

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 1.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:16:PHE:CE1 | 1:B:17:HIS:CE1 | 0.60 | 2.90 | 20 | 2 |
| 1:B:19:TYR:CE1 | 1:B:37:LEU:CB | 0.53 | 2.92 | 5 | 1 |
| 1:B:16:PHE:CZ | 1:B:17:HIS:CE1 | 0.51 | 2.99 | 6 | 1 |
| 1:A:38:ILE:HA | 1:A:41:GLU:HB3 | 0.46 | 1.87 | 16 | 2 |
| 1:B:16:PHE:CE2 | 1:B:17:HIS:CE1 | 0.45 | 3.05 | 1 | 1 |
| 1:B:19:TYR:CE1 | 1:B:37:LEU:HB2 | 0.45 | 2.45 | 5 | 1 |
| 1:A:31:LYS:NZ | 1:A:67:GLU:OE2 | 0.44 | 2.51 | 18 | 2 |
| 1:B:34:LEU:HD11 | 1:B:76:PHE:CE2 | 0.43 | 2.48 | 19 | 1 |
| 1:A:19:TYR:CD2 | 1:A:37:LEU:HD12 | 0.43 | 2.48 | 8 | 1 |
| 1:A:32:LYS:NZ | 1:A:33:GLU:OE2 | 0.43 | 2.52 | 20 | 1 |
| 1:B:32:LYS:NZ | 1:B:33:GLU:OE2 | 0.43 | 2.51 | 4 | 1 |
| 1:A:35:LYS:NZ | 1:A:59:ASP:OD1 | 0.42 | 2.52 | 1 | 1 |
| 1:B:58:ASP:C | 1:B:60:LEU:H | 0.42 | 2.17 | 19 | 3 |
| 1:B:38:ILE:HA | 1:B:41:GLU:HB3 | 0.42 | 1.91 | 18 | 1 |
| 1:B:40:LYS:NZ | 1:B:41:GLU:OE2 | 0.42 | 2.53 | 15 | 1 |
| 1:A:60:LEU:C | 1:A:62:ARG:H | 0.41 | 2.17 | 22 | 1 |
| 1:A:58:ASP:C | 1:A:60:LEU:H | 0.41 | 2.17 | 13 | 2 |
| 1:B:42:LEU:HD12 | 1:B:43:THR:H | 0.41 | 1.75 | 20 | 1 |
| 1:A:61:ASP:OD1 | 1:A:64:LYS:NZ | 0.41 | 2.52 | 22 | 1 |
| 1:A:32:LYS:NZ | 1:A:33:GLU:OE1 | 0.41 | 2.54 | 16 | 1 |
| 1:B:19:TYR:CD2 | 1:B:37:LEU:HD12 | 0.41 | 2.50 | 20 | 1 |
| 1:A:41:GLU:CG | 1:A:42:LEU:H | 0.41 | 2.27 | 16 | 1 |
| 1:A:84:TYR:O | 1:A:84:TYR:CG | 0.41 | 2.74 | 19 | 1 |
| 1:B:34:LEU:HD23 | 1:B:68:VAL:HG21 | 0.41 | 1.91 | 1 | 1 |
| 1:A:40:LYS:NZ | 1:A:41:GLU:OE2 | 0.41 | 2.54 | 20 | 2 |
| 1:A:64:LYS:NZ | 1:A:72:GLU:OE2 | 0.40 | 2.52 | 1 | 1 |
| 1:A:16:PHE:CZ | 1:A:17:HIS:CE1 | 0.40 | 3.10 | 21 | 1 |
| 1:A:16:PHE:CE2 | 1:A:17:HIS:CE1 | 0.40 | 3.10 | 21 | 1 |
| 1:B:64:LYS:NZ | 1:B:65:ASP:OD1 | 0.40 | 2.53 | 2 | 1 |
| 1:B:35:LYS:NZ | 1:B:59:ASP:OD2 | 0.40 | 2.55 | 17 | 1 |
| 1:B:61:ASP:OD1 | 1:B:64:LYS:NZ | 0.40 | 2.53 | 18 | 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 | 62/90 (69%) | 45±3 (72±5%) | 13±2 (20±4%) | 5±2 (8±3%) | 2 15 |
| 1 | B | 63/90 (70%) | 46±2 (72±3%) | 12±2 (19±4%) | 5±2 (8±3%) | 2 13 |
| All | All | 2750/3960 (69%) | 1985 (72%) | 549 (20%) | 216 (8%) | 2 14 |

All 55 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 59 | ASP | 9 |
| 1 | A | 63 | ASN | 8 |
| 1 | A | 86 | GLU | 8 |
| 1 | B | 31 | LYS | 8 |
| 1 | B | 43 | THR | 8 |
| 1 | A | 59 | ASP | 7 |
| 1 | B | 44 | ILE | 7 |
| 1 | B | 65 | ASP | 7 |
| 1 | A | 62 | ARG | 7 |
| 1 | B | 16 | PHE | 7 |
| 1 | B | 62 | ARG | 7 |
| 1 | A | 16 | PHE | 7 |
| 1 | B | 60 | LEU | 6 |
| 1 | A | 31 | LYS | 6 |
| 1 | B | 86 | GLU | 6 |
| 1 | A | 65 | ASP | 6 |
| 1 | B | 63 | ASN | 6 |
| 1 | A | 42 | LEU | 5 |
| 1 | A | 44 | ILE | 5 |
| 1 | B | 42 | LEU | 5 |
| 1 | A | 38 | ILE | 5 |
| 1 | B | 26 | LYS | 5 |
| 1 | A | 66 | GLN | 4 |
| 1 | B | 20 | SER | 4 |
| 1 | B | 64 | LYS | 4 |
| 1 | B | 66 | GLN | 4 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 41 | GLU | 4 |
| 1 | A | 20 | SER | 3 |
| 1 | A | 27 | HIS | 3 |
| 1 | A | 68 | VAL | 3 |
| 1 | B | 85 | ASN | 3 |
| 1 | A | 60 | LEU | 3 |
| 1 | A | 43 | THR | 3 |
| 1 | A | 30 | SER | 3 |
| 1 | B | 32 | LYS | 2 |
| 1 | A | 67 | GLU | 2 |
| 1 | B | 27 | HIS | 2 |
| 1 | B | 67 | GLU | 2 |
| 1 | B | 45 | GLY | 2 |
| 1 | A | 28 | THR | 2 |
| 1 | B | 38 | ILE | 2 |
| 1 | B | 41 | GLU | 2 |
| 1 | B | 83 | ILE | 2 |
| 1 | B | 30 | SER | 1 |
| 1 | B | 28 | THR | 1 |
| 1 | A | 17 | HIS | 1 |
| 1 | A | 14 | GLY | 1 |
| 1 | A | 71 | GLN | 1 |
| 1 | A | 37 | LEU | 1 |
| 1 | A | 39 | GLN | 1 |
| 1 | A | 85 | ASN | 1 |
| 1 | A | 81 | ALA | 1 |
| 1 | A | 61 | ASP | 1 |
| 1 | A | 64 | LYS | 1 |
| 1 | B | 21 | GLY | 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 | 57/77 (74%) | 47±3 (82±5%) | 10±3 (18±5%) | 4 38 |
| 1 | B | 55/77 (71%) | 46±2 (83±4%) | 9±2 (17±4%) | 5 40 |
| All | All | 2464/3388 (73%) | 2034 (83%) | 430 (17%) | 4 39 |

All 87 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 | 85 | ASN | 13 |
| 1 | B | 64 | LYS | 13 |
| 1 | A | 17 | HIS | 13 |
| 1 | A | 84 | TYR | 13 |
| 1 | B | 84 | TYR | 11 |
| 1 | B | 17 | HIS | 11 |
| 1 | A | 32 | LYS | 10 |
| 1 | B | 85 | ASN | 10 |
| 1 | A | 77 | LEU | 10 |
| 1 | A | 71 | GLN | 9 |
| 1 | A | 31 | LYS | 9 |
| 1 | A | 67 | GLU | 9 |
| 1 | A | 18 | LYS | 8 |
| 1 | A | 62 | ARG | 8 |
| 1 | B | 32 | LYS | 8 |
| 1 | B | 86 | GLU | 8 |
| 1 | A | 64 | LYS | 8 |
| 1 | A | 28 | THR | 7 |
| 1 | A | 69 | ASN | 7 |
| 1 | B | 61 | ASP | 7 |
| 1 | B | 77 | LEU | 7 |
| 1 | A | 26 | LYS | 7 |
| 1 | B | 62 | ARG | 7 |
| 1 | B | 26 | LYS | 6 |
| 1 | B | 34 | LEU | 6 |
| 1 | B | 76 | PHE | 6 |
| 1 | B | 18 | LYS | 6 |
| 1 | B | 28 | THR | 6 |
| 1 | B | 43 | THR | 6 |
| 1 | B | 69 | ASN | 6 |
| 1 | A | 35 | LYS | 6 |
| 1 | A | 59 | ASP | 6 |
| 1 | B | 35 | LYS | 6 |
| 1 | B | 71 | GLN | 6 |
| 1 | A | 40 | LYS | 6 |
| 1 | A | 61 | ASP | 6 |
| 1 | A | 42 | LEU | 5 |
| 1 | A | 76 | PHE | 5 |
| 1 | B | 42 | LEU | 5 |
| 1 | A | 34 | LEU | 5 |
| 1 | A | 58 | ASP | 5 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 36 | GLU | 5 |
| 1 | B | 66 | GLN | 5 |
| 1 | A | 65 | ASP | 4 |
| 1 | B | 58 | ASP | 4 |
| 1 | A | 86 | GLU | 4 |
| 1 | B | 37 | LEU | 4 |
| 1 | A | 16 | PHE | 4 |
| 1 | A | 38 | ILE | 4 |
| 1 | A | 73 | TYR | 4 |
| 1 | B | 31 | LYS | 4 |
| 1 | B | 40 | LYS | 4 |
| 1 | B | 41 | GLU | 4 |
| 1 | A | 27 | HIS | 4 |
| 1 | A | 41 | GLU | 4 |
| 1 | B | 67 | GLU | 3 |
| 1 | B | 30 | SER | 3 |
| 1 | B | 65 | ASP | 3 |
| 1 | A | 63 | ASN | 3 |
| 1 | B | 38 | ILE | 3 |
| 1 | B | 13 | ILE | 3 |
| 1 | B | 72 | GLU | 3 |
| 1 | B | 16 | PHE | 2 |
| 1 | B | 59 | ASP | 2 |
| 1 | A | 37 | LEU | 2 |
| 1 | B | 33 | GLU | 2 |
| 1 | A | 29 | LEU | 2 |
| 1 | A | 39 | GLN | 2 |
| 1 | B | 73 | TYR | 2 |
| 1 | A | 82 | MET | 2 |
| 1 | A | 72 | GLU | 2 |
| 1 | B | 27 | HIS | 2 |
| 1 | A | 43 | THR | 1 |
| 1 | B | 82 | MET | 1 |
| 1 | A | 36 | GLU | 1 |
| 1 | B | 29 | LEU | 1 |
| 1 | A | 11 | LEU | 1 |
| 1 | A | 75 | THR | 1 |
| 1 | B | 68 | VAL | 1 |
| 1 | A | 68 | VAL | 1 |
| 1 | B | 15 | ILE | 1 |
| 1 | A | 44 | ILE | 1 |
| 1 | B | 44 | ILE | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 11 | LEU | 1 |
| 1 | A | 30 | SER | 1 |
| 1 | A | 74 | ILE | 1 |
| 1 | B | 70 | PHE | 1 |

#### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry (i)

There are no ligands in this entry.

### 6.7 Other polymers (i)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

No chemical shift data were provided