



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2023 – 02:55 PM EDT

PDB ID : 2Q4P  
Title : Ensemble refinement of the crystal structure of protein from *Mus musculus* Mm.29898  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.32 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

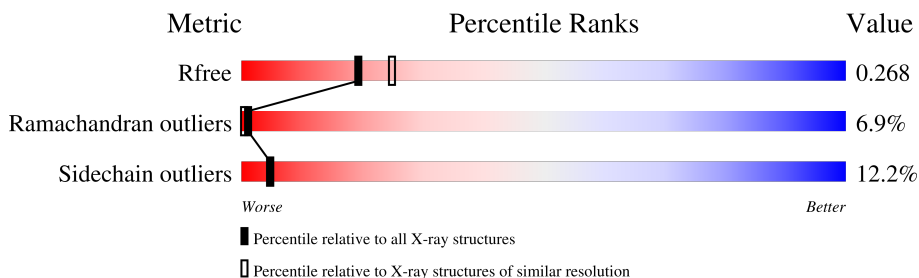
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 Å.

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.




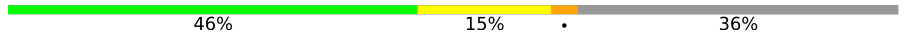

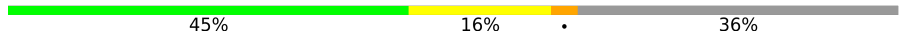

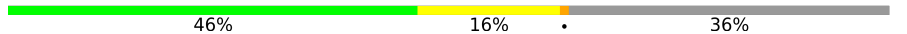
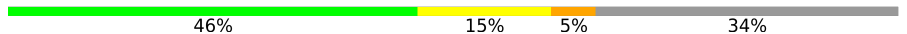
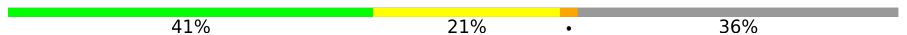
















| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 5974 (2.34-2.30)                                      |
| Ramachandran outliers | 138981                      | 6523 (2.34-2.30)                                      |
| Sidechain outliers    | 138945                      | 6523 (2.34-2.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1-A   | 170    |                  |
| 1   | 1-B   | 170    |                  |
| 1   | 10-A  | 170    |                  |
| 1   | 10-B  | 170    |                  |
| 1   | 11-A  | 170    |                  |
| 1   | 11-B  | 170    |                  |
| 1   | 12-A  | 170    |                  |
| 1   | 12-B  | 170    |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 13-A  | 170    |  52% 14% 34%    |
| 1   | 13-B  | 170    |  46% 15% 36%    |
| 1   | 14-A  | 170    |  49% 16% 34%    |
| 1   | 14-B  | 170    |  45% 16% 36%    |
| 1   | 15-A  | 170    |  52% 14% 34%    |
| 1   | 15-B  | 170    |  46% 16% 36%    |
| 1   | 16-A  | 170    |  46% 15% 5% 34% |
| 1   | 16-B  | 170    |  41% 21% 36%    |
| 1   | 2-A   | 170    |  55% 11% 34%    |
| 1   | 2-B   | 170    |  54% 9% 36%     |
| 1   | 3-A   | 170    |  59% 6% 34%     |
| 1   | 3-B   | 170    |  58% 6% 36%    |
| 1   | 4-A   | 170    |  58% 8% 34%   |
| 1   | 4-B   | 170    |  53% 10% 36%  |
| 1   | 5-A   | 170    |  58% 8% 34%   |
| 1   | 5-B   | 170    |  54% 9% 36%   |
| 1   | 6-A   | 170    |  58% 8% 34%   |
| 1   | 6-B   | 170    |  53% 11% 36%  |
| 1   | 7-A   | 170    |  58% 7% 34%   |
| 1   | 7-B   | 170    |  53% 10% 36%  |
| 1   | 8-A   | 170    |  59% 8% 34%   |
| 1   | 8-B   | 170    |  52% 11% 36%  |
| 1   | 9-A   | 170    |  54% 11% 34%  |
| 1   | 9-B   | 170    |  57% 6% 36%   |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29392 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein RS21-C6.

| Mol | Chain | Residues | Atoms |     |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S | Se |         |         |       |
| 1   | 1-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 2-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 3-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 4-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 5-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 6-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 7-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 8-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 9-A   | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 10-A  | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 11-A  | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 12-A  | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 13-A  | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 14-A  | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 15-A  | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |
| 1   | 16-A  | 113      | 922   | 589 | 163 | 168 | 1 | 1  | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S | Se |         |         |       |
| 1   | 1-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 2-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 3-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 4-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 5-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 6-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 7-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 8-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 9-B   | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 10-B  | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 11-B  | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 12-B  | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 13-B  | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 14-B  | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 15-B  | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |
| 1   | 16-B  | 109      | 891   | 569 | 157 | 163 | 1 | 1  | 0       | 0       | 0     |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | MSE      | MET    | modified residue | UNP Q9QY93 |
| A     | 122     | MSE      | MET    | modified residue | UNP Q9QY93 |
| B     | 1       | MSE      | MET    | modified residue | UNP Q9QY93 |
| B     | 122     | MSE      | MET    | modified residue | UNP Q9QY93 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2   | 1-A   | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 2-A   | 11       | Total O<br>11 11 | 0       | 0       |
| 2   | 3-A   | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 4-A   | 11       | Total O<br>11 11 | 0       | 0       |
| 2   | 5-A   | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 6-A   | 11       | Total O<br>11 11 | 0       | 0       |
| 2   | 7-A   | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 8-A   | 13       | Total O<br>13 13 | 0       | 0       |
| 2   | 9-A   | 11       | Total O<br>11 11 | 0       | 0       |
| 2   | 10-A  | 10       | Total O<br>10 10 | 0       | 0       |
| 2   | 11-A  | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 12-A  | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 13-A  | 13       | Total O<br>13 13 | 0       | 0       |
| 2   | 14-A  | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 15-A  | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 16-A  | 13       | Total O<br>13 13 | 0       | 0       |
| 2   | 1-B   | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 2-B   | 13       | Total O<br>13 13 | 0       | 0       |
| 2   | 3-B   | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 4-B   | 13       | Total O<br>13 13 | 0       | 0       |
| 2   | 5-B   | 12       | Total O<br>12 12 | 0       | 0       |
| 2   | 6-B   | 13       | Total O<br>13 13 | 0       | 0       |

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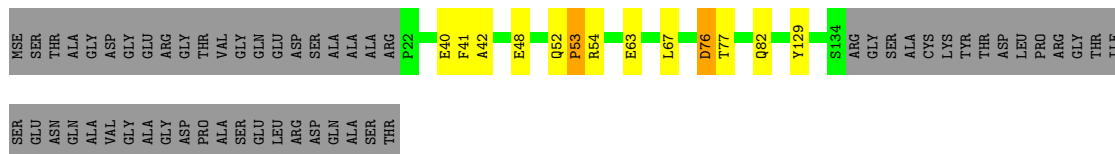
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| <b>Mol</b> | <b>Chain</b> | <b>Residues</b> | <b>Atoms</b>     | <b>ZeroOcc</b> | <b>AltConf</b> |
|------------|--------------|-----------------|------------------|----------------|----------------|
| 2          | 7-B          | 12              | Total O<br>12 12 | 0              | 0              |
| 2          | 8-B          | 11              | Total O<br>11 11 | 0              | 0              |
| 2          | 9-B          | 13              | Total O<br>13 13 | 0              | 0              |
| 2          | 10-B         | 14              | Total O<br>14 14 | 0              | 0              |
| 2          | 11-B         | 12              | Total O<br>12 12 | 0              | 0              |
| 2          | 12-B         | 12              | Total O<br>12 12 | 0              | 0              |
| 2          | 13-B         | 11              | Total O<br>11 11 | 0              | 0              |
| 2          | 14-B         | 12              | Total O<br>12 12 | 0              | 0              |
| 2          | 15-B         | 12              | Total O<br>12 12 | 0              | 0              |
| 2          | 16-B         | 11              | Total O<br>11 11 | 0              | 0              |



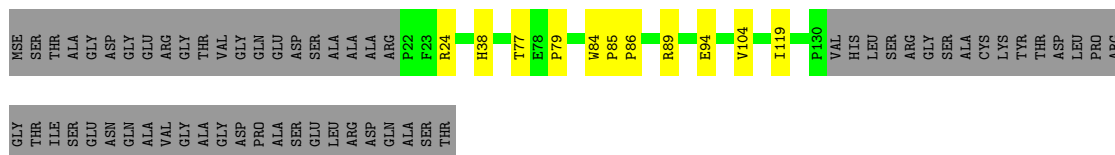


Chain 3-A:  59% 6% 34%



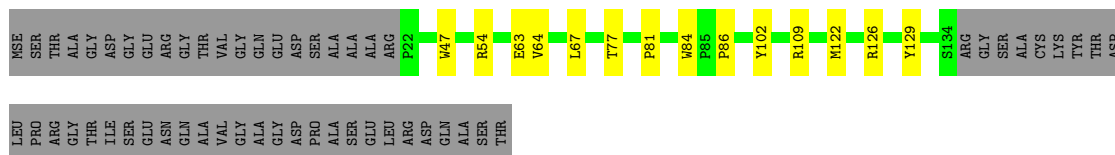
• Molecule 1: Protein RS21-C6

Chain 3-B:  58% 6% 36%



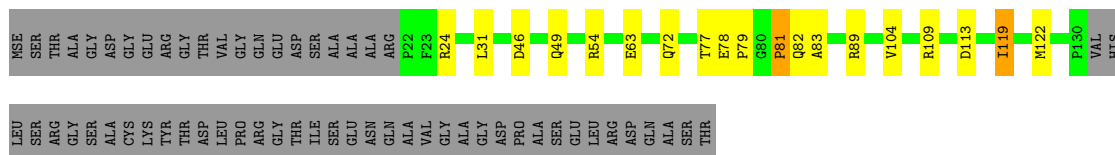
• Molecule 1: Protein RS21-C6

Chain 4-A:  58% 8% 34%



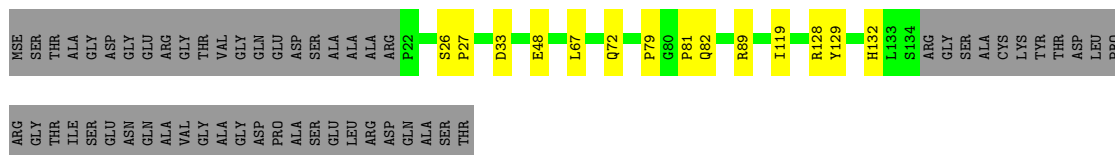
• Molecule 1: Protein RS21-C6

Chain 4-B:  53% 10% 36%



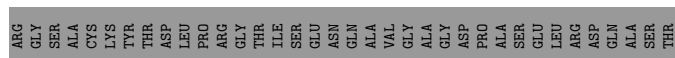
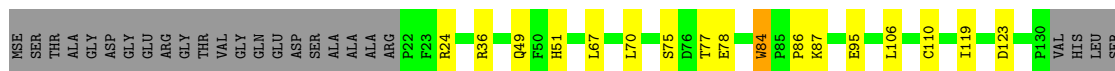
• Molecule 1: Protein RS21-C6

Chain 5-A:  58% 8% 34%

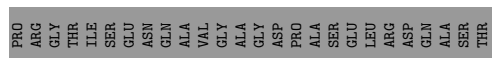


• Molecule 1: Protein RS21-C6

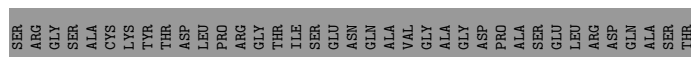
Chain 5-B:  54% 9% 36%



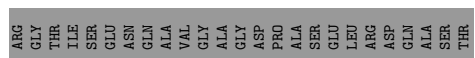
• Molecule 1: Protein RS21-C6



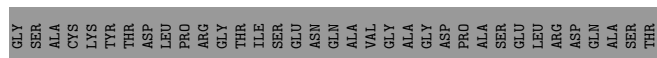
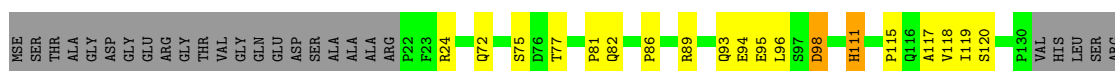
• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6



GLY  
THR  
ILE  
SER  
GLU  
ASN  
GLN  
VAL  
ALA  
GLY  
GLY  
ASP  
PRO  
ALA  
SER  
SER  
GLU  
LEU  
LEU  
ARG  
ASP  
GLN  
ALA  
SER  
THR

- Molecule 1: Protein RS21-C6

Chain 8-B: 52% 11% 36%

MSE  
SER  
THR  
ALA  
GLY  
ASP  
GLY  
GLU  
ARG  
THR  
THR  
GLY  
GLN  
ASP  
SER  
GLU  
ALA  
ALA  
ALA  
P22  
D33  
R36  
L37  
R45  
F50  
L56  
L60  
E63  
L67  
A68  
E69  
Q72  
P85  
P86  
K87  
Q93  
E94  
E95  
H111  
V112  
D113  
L114  
D123  
Q127

P130  
VAL  
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SER  
ARG  
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ARG  
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CYS  
GLY  
TYR  
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GLU  
GLN  
ASP  
LEU  
SER  
PRO  
ARG  
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GLY  
THR  
THR  
ILE  
SER  
SER  
GLU  
PRO  
ASN  
GLN  
ALA  
VAL  
ALA  
ALA  
ALA  
ALA  
THR

- Molecule 1: Protein RS21-C6

Chain 9-A: 54% 11% 34%

MSE  
SER  
THR  
ALA  
GLY  
ASP  
GLY  
GLU  
ARG  
THR  
THR  
VAL  
GLY  
GLN  
GLU  
ASP  
SER  
SER  
ALA  
VAL  
ALA  
ALA  
ALA  
ARG  
P22  
F23  
D46  
W47  
E48  
F71  
Q72  
E78  
Q82  
P86  
K87  
E88  
Q93  
E94  
E95  
D98  
Y99  
L100  
P115  
I119  
M122  
D123  
Y129  
S134  
ARG  
GLY  
SER

ALA  
CYS  
LYS  
TYR  
THR  
THR  
ASP  
LEU  
PRO  
ARG  
GLY  
THR  
THR  
ILE  
SER  
SER  
GLU  
GLN  
ASP  
PRO  
ASN  
GLN  
ALA  
VAL  
ALA  
ALA  
ALA  
GLY  
THR  
THR

- Molecule 1: Protein RS21-C6

Chain 9-B: 57% 6% 36%

MSE  
SER  
THR  
ALA  
GLY  
ASP  
GLY  
GLU  
ARG  
THR  
THR  
VAL  
GLY  
GLN  
GLU  
ASP  
SER  
SER  
ALA  
VAL  
ALA  
ALA  
ALA  
ARG  
P22  
F23  
R36  
D46  
Q49  
L67  
Q72  
S75  
E78  
P85  
R89  
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SER  
SER  
ARG  
GLY  
SER  
SER  
ALA  
ALA  
CYS  
LYS  
TYR  
THR  
ASP  
LEU

PRO  
ARG  
GLY  
THR  
ILE  
SER  
GLU  
ASN  
GLN  
ALA  
VAL  
GLY  
ALA  
GLY  
GLN  
ASP  
PRO  
ASN  
SER  
SER  
ALA  
VAL  
LEU  
LEU  
ARG  
ASP  
ALA  
SER  
THR

- Molecule 1: Protein RS21-C6

Chain 10-A: 55% 9% 34%

MSE  
SER  
THR  
ALA  
GLY  
ASP  
GLY  
GLU  
ARG  
THR  
THR  
VAL  
GLY  
GLN  
GLU  
ASP  
SER  
SER  
ALA  
VAL  
ALA  
ALA  
ARG  
P22  
F23  
R24  
E28  
L37  
D46  
W47  
E48  
V64  
Q72  
S75  
E78  
P81  
Q82  
A83  
W84  
P85  
P86  
Q93  
E94  
E95  
Y102  
Y129  
H132  
L133  
S134  
ARG

GLY  
SER  
ALA  
CYS  
LYS  
TYR  
THR  
THR  
ASP  
LEU  
PRO  
ARG  
THR  
THR  
ILE  
SER  
SER  
GLU  
GLN  
ASN  
SER  
SER  
ALA  
VAL  
VAL  
VAL  
GLY  
GLY  
ASP  
PRO  
ASN  
GLN  
ALA  
VAL  
ALA  
ALA  
THR

- Molecule 1: Protein RS21-C6

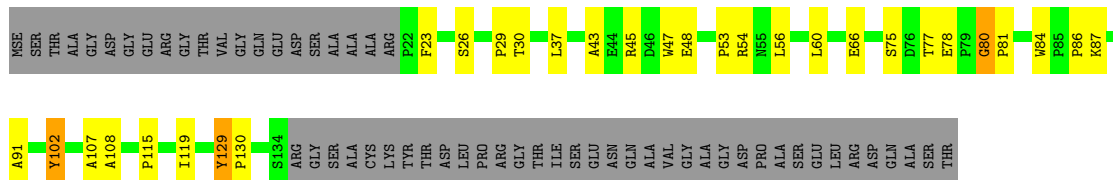
Chain 10-B: 54% 10% 36%

MSE  
SER  
THR  
ALA  
GLY  
ASP  
GLY  
GLU  
ARG  
THR  
THR  
VAL  
GLY  
GLN  
GLU  
ASP  
SER  
SER  
ALA  
VAL  
ALA  
ALA  
ARG  
P22  
F25  
S26  
F27  
E28  
P29  
T30  
D33  
W73  
K74  
S75  
T77  
E78  
P86  
D98  
V104  
Q116  
M122  
D123  
T124  
H125  
R126  
P130  
VAL  
HIS  
LEU  
SER  
ARG  
GLY

SER  
ALA  
CYS  
LYS  
TYR  
THR  
THR  
ASP  
LEU  
PRO  
ARG  
THR  
THR  
ILE  
SER  
SER  
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ASN  
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SER  
ALA  
VAL  
VAL  
VAL  
GLY  
GLY  
ASP  
PRO  
ASN  
GLN  
ALA  
VAL  
ALA  
ALA  
THR

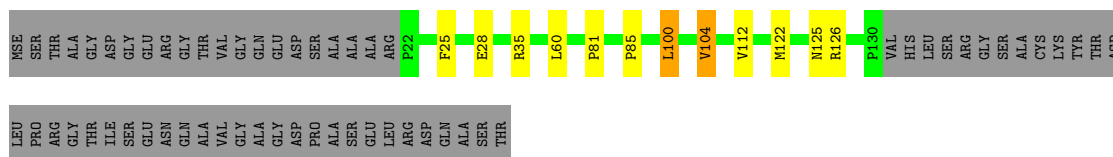
- Molecule 1: Protein RS21-C6

Chain 11-A:  49% 16% 34%



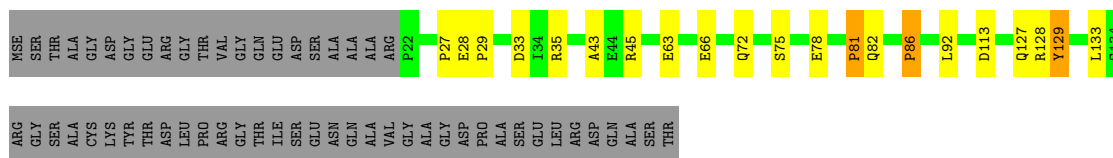
- Molecule 1: Protein RS21-C6

Chain 11-B:  57% 6% 36%



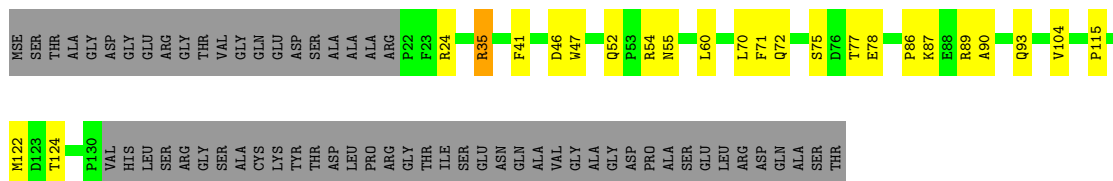
- Molecule 1: Protein RS21-C6

Chain 12-A:  54% 11% 34%



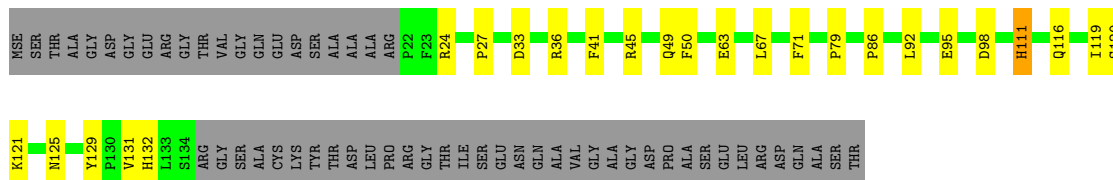
- Molecule 1: Protein RS21-C6

Chain 12-B:  50% 14% 36%

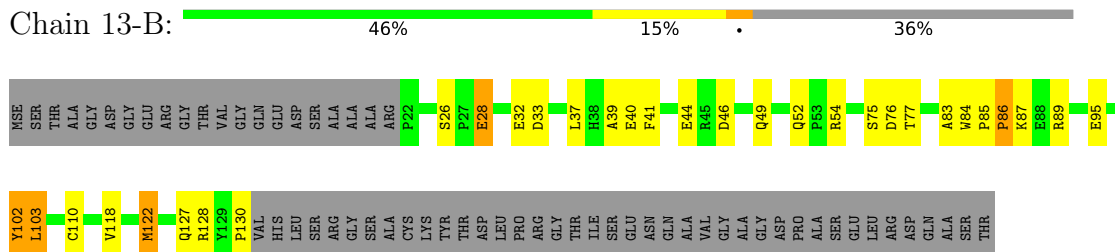


- Molecule 1: Protein RS21-C6

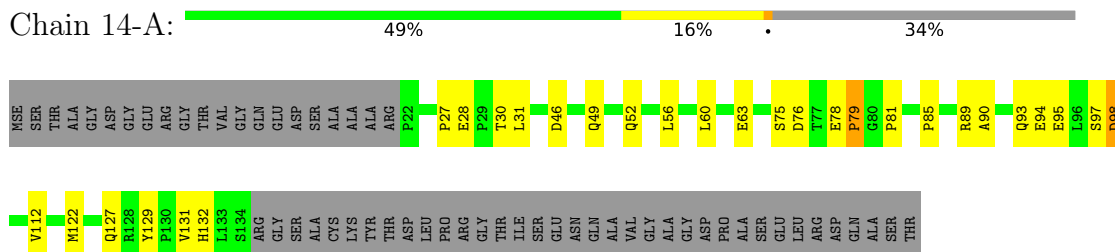
Chain 13-A:  52% 14% 34%



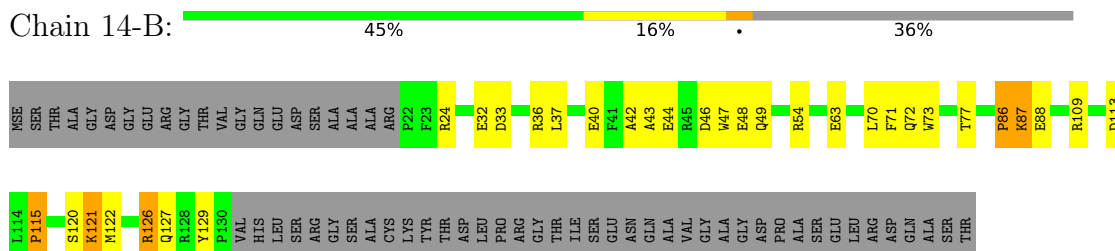
- Molecule 1: Protein RS21-C6



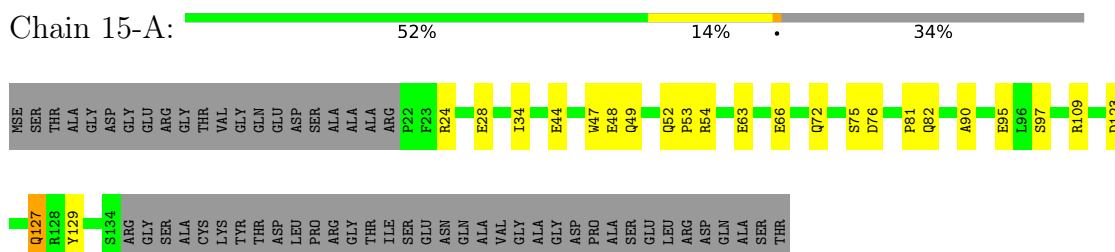
• Molecule 1: Protein RS21-C6



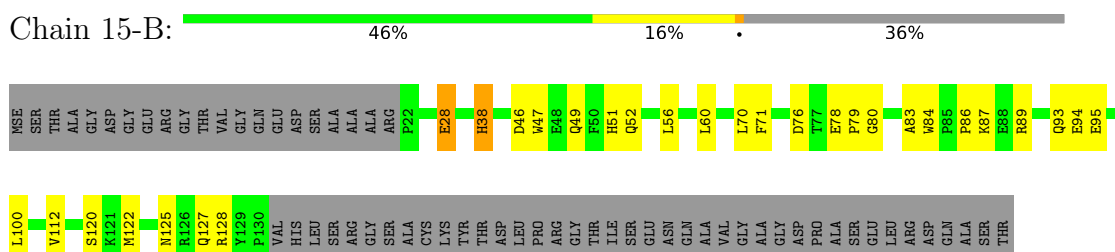
• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6



• Molecule 1: Protein RS21-C6



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 65 2 2  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 73.54Å 73.54Å 236.08Å<br>90.00° 90.00° 120.00°              | Depositor        |
| Resolution (Å)  | 37.93 – 2.32<br>43.29 – 2.32                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.3 (37.93-2.32)<br>98.5 (43.29-2.32)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.69 (at 2.32Å)   | Xtrriage         |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.138 , 0.233<br>0.192 , 0.268                              | Depositor<br>DCC |
| $R_{free}$ test set   | 858 reflections (5.07%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 55.5  | Xtrriage         |
| Anisotropy  | 0.134   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.40 , 652.5  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 29392   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 46.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 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 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   | 1-A   | 0.83         | 0/947           | 1.09        | 1/1288 (0.1%)   |
| 1   | 1-B   | 0.93         | 0/915           | 1.02        | 2/1244 (0.2%)   |
| 1   | 2-A   | 0.92         | 0/947           | 1.08        | 2/1288 (0.2%)   |
| 1   | 2-B   | 0.94         | 1/915 (0.1%)    | 1.01        | 1/1244 (0.1%)   |
| 1   | 3-A   | 0.87         | 0/947           | 0.94        | 0/1288          |
| 1   | 3-B   | 0.99         | 0/915           | 0.95        | 0/1244          |
| 1   | 4-A   | 0.94         | 0/947           | 0.98        | 0/1288          |
| 1   | 4-B   | 1.01         | 0/915           | 1.11        | 3/1244 (0.2%)   |
| 1   | 5-A   | 0.89         | 0/947           | 0.91        | 0/1288          |
| 1   | 5-B   | 0.93         | 1/915 (0.1%)    | 0.98        | 3/1244 (0.2%)   |
| 1   | 6-A   | 0.87         | 0/947           | 0.98        | 0/1288          |
| 1   | 6-B   | 1.05         | 2/915 (0.2%)    | 1.11        | 4/1244 (0.3%)   |
| 1   | 7-A   | 0.90         | 0/947           | 0.99        | 2/1288 (0.2%)   |
| 1   | 7-B   | 0.92         | 0/915           | 0.98        | 1/1244 (0.1%)   |
| 1   | 8-A   | 0.86         | 0/947           | 0.99        | 1/1288 (0.1%)   |
| 1   | 8-B   | 0.99         | 2/915 (0.2%)    | 1.09        | 2/1244 (0.2%)   |
| 1   | 9-A   | 0.94         | 2/947 (0.2%)    | 0.98        | 0/1288          |
| 1   | 9-B   | 0.90         | 0/915           | 0.94        | 1/1244 (0.1%)   |
| 1   | 10-A  | 0.93         | 1/947 (0.1%)    | 1.01        | 2/1288 (0.2%)   |
| 1   | 10-B  | 0.98         | 0/915           | 1.04        | 4/1244 (0.3%)   |
| 1   | 11-A  | 0.95         | 1/947 (0.1%)    | 1.12        | 7/1288 (0.5%)   |
| 1   | 11-B  | 0.99         | 1/915 (0.1%)    | 1.22        | 4/1244 (0.3%)   |
| 1   | 12-A  | 0.96         | 1/947 (0.1%)    | 1.02        | 2/1288 (0.2%)   |
| 1   | 12-B  | 0.91         | 1/915 (0.1%)    | 1.07        | 3/1244 (0.2%)   |
| 1   | 13-A  | 1.05         | 0/947           | 1.15        | 2/1288 (0.2%)   |
| 1   | 13-B  | 1.28         | 5/915 (0.5%)    | 1.26        | 7/1244 (0.6%)   |
| 1   | 14-A  | 1.05         | 1/947 (0.1%)    | 1.23        | 4/1288 (0.3%)   |
| 1   | 14-B  | 1.10         | 2/915 (0.2%)    | 1.13        | 3/1244 (0.2%)   |
| 1   | 15-A  | 0.98         | 1/947 (0.1%)    | 1.10        | 2/1288 (0.2%)   |
| 1   | 15-B  | 1.16         | 2/915 (0.2%)    | 1.16        | 4/1244 (0.3%)   |
| 1   | 16-A  | 1.11         | 2/947 (0.2%)    | 1.31        | 10/1288 (0.8%)  |
| 1   | 16-B  | 1.39         | 9/915 (1.0%)    | 1.41        | 13/1244 (1.0%)  |
| All | All   | 0.99         | 35/29792 (0.1%) | 1.08        | 90/40512 (0.2%) |



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 outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 5-B   | 0                   | 1                   |
| 1   | 9-A   | 0                   | 1                   |
| 1   | 11-A  | 0                   | 1                   |
| 1   | 12-A  | 0                   | 1                   |
| 1   | 13-B  | 0                   | 2                   |
| 1   | 16-A  | 0                   | 1                   |
| 1   | 16-B  | 0                   | 1                   |
| All | All   | 0                   | 8                   |

The worst 5 of 35 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 16-B  | 42  | ALA  | CA-CB  | 13.50 | 1.80        | 1.52     |
| 1   | 16-B  | 28  | GLU  | CD-OE1 | -8.05 | 1.16        | 1.25     |
| 1   | 16-B  | 28  | GLU  | CG-CD  | 7.98  | 1.64        | 1.51     |
| 1   | 13-B  | 39  | ALA  | CA-CB  | -7.26 | 1.37        | 1.52     |
| 1   | 14-A  | 94  | GLU  | CG-CD  | 7.26  | 1.62        | 1.51     |

The worst 5 of 90 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | 11-B  | 35  | ARG  | NE-CZ-NH1 | 15.25  | 127.92      | 120.30   |
| 1   | 11-B  | 35  | ARG  | NE-CZ-NH2 | -14.82 | 112.89      | 120.30   |
| 1   | 12-B  | 35  | ARG  | NE-CZ-NH2 | -10.14 | 115.23      | 120.30   |
| 1   | 6-B   | 89  | ARG  | NE-CZ-NH1 | 8.72   | 124.66      | 120.30   |
| 1   | 5-B   | 36  | ARG  | NE-CZ-NH1 | 8.12   | 124.36      | 120.30   |

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 11-A  | 102 | TYR  | Sidechain |
| 1   | 12-A  | 129 | TYR  | Sidechain |
| 1   | 13-B  | 41  | PHE  | Sidechain |
| 1   | 5-B   | 51  | HIS  | Sidechain |
| 1   | 9-A   | 71  | PHE  | Sidechain |

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 1-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 2-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 2-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 3-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 3-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 4-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 4-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 5-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 5-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 6-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 6-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 7-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 7-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 8-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 8-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 9-A   | 922   | 0        | 901      | 0       | 0            |
| 1   | 9-B   | 891   | 0        | 869      | 0       | 0            |
| 1   | 10-A  | 922   | 0        | 901      | 0       | 0            |
| 1   | 10-B  | 891   | 0        | 869      | 0       | 0            |
| 1   | 11-A  | 922   | 0        | 901      | 0       | 0            |
| 1   | 11-B  | 891   | 0        | 869      | 0       | 0            |
| 1   | 12-A  | 922   | 0        | 901      | 0       | 0            |
| 1   | 12-B  | 891   | 0        | 869      | 0       | 0            |
| 1   | 13-A  | 922   | 0        | 901      | 0       | 0            |
| 1   | 13-B  | 891   | 0        | 869      | 0       | 0            |
| 1   | 14-A  | 922   | 0        | 901      | 0       | 0            |
| 1   | 14-B  | 891   | 0        | 869      | 0       | 0            |
| 1   | 15-A  | 922   | 0        | 901      | 0       | 0            |
| 1   | 15-B  | 891   | 0        | 869      | 0       | 0            |
| 1   | 16-A  | 922   | 0        | 901      | 0       | 0            |
| 1   | 16-B  | 891   | 0        | 869      | 0       | 0            |
| 2   | 1-A   | 12    | 0        | 0        | 0       | 0            |
| 2   | 1-B   | 12    | 0        | 0        | 0       | 0            |
| 2   | 2-A   | 11    | 0        | 0        | 0       | 0            |
| 2   | 2-B   | 13    | 0        | 0        | 0       | 0            |
| 2   | 3-A   | 12    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 3-B   | 12    | 0        | 0        | 0       | 0            |
| 2   | 4-A   | 11    | 0        | 0        | 0       | 0            |
| 2   | 4-B   | 13    | 0        | 0        | 0       | 0            |
| 2   | 5-A   | 12    | 0        | 0        | 0       | 0            |
| 2   | 5-B   | 12    | 0        | 0        | 0       | 0            |
| 2   | 6-A   | 11    | 0        | 0        | 0       | 0            |
| 2   | 6-B   | 13    | 0        | 0        | 0       | 0            |
| 2   | 7-A   | 12    | 0        | 0        | 0       | 0            |
| 2   | 7-B   | 12    | 0        | 0        | 0       | 0            |
| 2   | 8-A   | 13    | 0        | 0        | 0       | 0            |
| 2   | 8-B   | 11    | 0        | 0        | 0       | 0            |
| 2   | 9-A   | 11    | 0        | 0        | 0       | 0            |
| 2   | 9-B   | 13    | 0        | 0        | 0       | 0            |
| 2   | 10-A  | 10    | 0        | 0        | 0       | 0            |
| 2   | 10-B  | 14    | 0        | 0        | 0       | 0            |
| 2   | 11-A  | 12    | 0        | 0        | 0       | 0            |
| 2   | 11-B  | 12    | 0        | 0        | 0       | 0            |
| 2   | 12-A  | 12    | 0        | 0        | 0       | 0            |
| 2   | 12-B  | 12    | 0        | 0        | 0       | 0            |
| 2   | 13-A  | 13    | 0        | 0        | 0       | 0            |
| 2   | 13-B  | 11    | 0        | 0        | 0       | 0            |
| 2   | 14-A  | 12    | 0        | 0        | 0       | 0            |
| 2   | 14-B  | 12    | 0        | 0        | 0       | 0            |
| 2   | 15-A  | 12    | 0        | 0        | 0       | 0            |
| 2   | 15-B  | 12    | 0        | 0        | 0       | 0            |
| 2   | 16-A  | 13    | 0        | 0        | 0       | 0            |
| 2   | 16-B  | 11    | 0        | 0        | 0       | 0            |
| All | All   | 29392 | 0        | 28320    | 0       | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | 1-A   | 111/170 (65%) | 83 (75%) | 23 (21%) | 5 (4%)   | 2           | 1 |
| 1   | 1-B   | 107/170 (63%) | 83 (78%) | 22 (21%) | 2 (2%)   | 8           | 6 |
| 1   | 2-A   | 111/170 (65%) | 89 (80%) | 18 (16%) | 4 (4%)   | 3           | 2 |
| 1   | 2-B   | 107/170 (63%) | 90 (84%) | 10 (9%)  | 7 (6%)   | 1           | 0 |
| 1   | 3-A   | 111/170 (65%) | 97 (87%) | 9 (8%)   | 5 (4%)   | 2           | 1 |
| 1   | 3-B   | 107/170 (63%) | 98 (92%) | 6 (6%)   | 3 (3%)   | 5           | 3 |
| 1   | 4-A   | 111/170 (65%) | 92 (83%) | 14 (13%) | 5 (4%)   | 2           | 1 |
| 1   | 4-B   | 107/170 (63%) | 85 (79%) | 14 (13%) | 8 (8%)   | 1           | 0 |
| 1   | 5-A   | 111/170 (65%) | 95 (86%) | 12 (11%) | 4 (4%)   | 3           | 2 |
| 1   | 5-B   | 107/170 (63%) | 98 (92%) | 6 (6%)   | 3 (3%)   | 5           | 3 |
| 1   | 6-A   | 111/170 (65%) | 91 (82%) | 13 (12%) | 7 (6%)   | 1           | 0 |
| 1   | 6-B   | 107/170 (63%) | 85 (79%) | 16 (15%) | 6 (6%)   | 2           | 0 |
| 1   | 7-A   | 111/170 (65%) | 85 (77%) | 18 (16%) | 8 (7%)   | 1           | 0 |
| 1   | 7-B   | 107/170 (63%) | 85 (79%) | 10 (9%)  | 12 (11%) | 0           | 0 |
| 1   | 8-A   | 111/170 (65%) | 96 (86%) | 12 (11%) | 3 (3%)   | 5           | 3 |
| 1   | 8-B   | 107/170 (63%) | 80 (75%) | 18 (17%) | 9 (8%)   | 1           | 0 |
| 1   | 9-A   | 111/170 (65%) | 80 (72%) | 22 (20%) | 9 (8%)   | 1           | 0 |
| 1   | 9-B   | 107/170 (63%) | 92 (86%) | 11 (10%) | 4 (4%)   | 3           | 1 |
| 1   | 10-A  | 111/170 (65%) | 90 (81%) | 16 (14%) | 5 (4%)   | 2           | 1 |
| 1   | 10-B  | 107/170 (63%) | 85 (79%) | 15 (14%) | 7 (6%)   | 1           | 0 |
| 1   | 11-A  | 111/170 (65%) | 79 (71%) | 17 (15%) | 15 (14%) | 0           | 0 |
| 1   | 11-B  | 107/170 (63%) | 87 (81%) | 14 (13%) | 6 (6%)   | 2           | 0 |
| 1   | 12-A  | 111/170 (65%) | 82 (74%) | 19 (17%) | 10 (9%)  | 1           | 0 |
| 1   | 12-B  | 107/170 (63%) | 75 (70%) | 22 (21%) | 10 (9%)  | 0           | 0 |
| 1   | 13-A  | 111/170 (65%) | 85 (77%) | 19 (17%) | 7 (6%)   | 1           | 0 |
| 1   | 13-B  | 107/170 (63%) | 82 (77%) | 16 (15%) | 9 (8%)   | 1           | 0 |
| 1   | 14-A  | 111/170 (65%) | 77 (69%) | 21 (19%) | 13 (12%) | 0           | 0 |
| 1   | 14-B  | 107/170 (63%) | 81 (76%) | 14 (13%) | 12 (11%) | 0           | 0 |
| 1   | 15-A  | 111/170 (65%) | 80 (72%) | 20 (18%) | 11 (10%) | 0           | 0 |
| 1   | 15-B  | 107/170 (63%) | 84 (78%) | 16 (15%) | 7 (6%)   | 1           | 0 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | 16-A  | 111/170 (65%)   | 75 (68%)   | 23 (21%)  | 13 (12%) | 0           | 0 |
| 1   | 16-B  | 107/170 (63%)   | 76 (71%)   | 19 (18%)  | 12 (11%) | 0           | 0 |
| All | All   | 3488/5440 (64%) | 2742 (79%) | 505 (14%) | 241 (7%) | 1           | 0 |

5 of 241 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 78  | GLU  |
| 1   | 1-A   | 128 | ARG  |
| 1   | 1-B   | 86  | PRO  |
| 1   | 2-A   | 81  | PRO  |
| 1   | 2-B   | 72  | GLN  |

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | 1-A   | 98/136 (72%) | 83 (85%)  | 15 (15%) | 2           | 2  |
| 1   | 1-B   | 94/136 (69%) | 84 (89%)  | 10 (11%) | 6           | 7  |
| 1   | 2-A   | 98/136 (72%) | 83 (85%)  | 15 (15%) | 2           | 2  |
| 1   | 2-B   | 94/136 (69%) | 85 (90%)  | 9 (10%)  | 8           | 9  |
| 1   | 3-A   | 98/136 (72%) | 88 (90%)  | 10 (10%) | 7           | 8  |
| 1   | 3-B   | 94/136 (69%) | 86 (92%)  | 8 (8%)   | 10          | 12 |
| 1   | 4-A   | 98/136 (72%) | 89 (91%)  | 9 (9%)   | 9           | 10 |
| 1   | 4-B   | 94/136 (69%) | 84 (89%)  | 10 (11%) | 6           | 7  |
| 1   | 5-A   | 98/136 (72%) | 88 (90%)  | 10 (10%) | 7           | 8  |
| 1   | 5-B   | 94/136 (69%) | 82 (87%)  | 12 (13%) | 4           | 4  |
| 1   | 6-A   | 98/136 (72%) | 89 (91%)  | 9 (9%)   | 9           | 10 |
| 1   | 6-B   | 94/136 (69%) | 85 (90%)  | 9 (10%)  | 8           | 9  |
| 1   | 7-A   | 98/136 (72%) | 89 (91%)  | 9 (9%)   | 9           | 10 |
| 1   | 7-B   | 94/136 (69%) | 86 (92%)  | 8 (8%)   | 10          | 12 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | 8-A   | 98/136 (72%)    | 89 (91%)   | 9 (9%)    | 9           | 10 |
| 1   | 8-B   | 94/136 (69%)    | 84 (89%)   | 10 (11%)  | 6           | 7  |
| 1   | 9-A   | 98/136 (72%)    | 87 (89%)   | 11 (11%)  | 6           | 6  |
| 1   | 9-B   | 94/136 (69%)    | 86 (92%)   | 8 (8%)    | 10          | 12 |
| 1   | 10-A  | 98/136 (72%)    | 84 (86%)   | 14 (14%)  | 3           | 3  |
| 1   | 10-B  | 94/136 (69%)    | 86 (92%)   | 8 (8%)    | 10          | 12 |
| 1   | 11-A  | 98/136 (72%)    | 88 (90%)   | 10 (10%)  | 7           | 8  |
| 1   | 11-B  | 94/136 (69%)    | 90 (96%)   | 4 (4%)    | 29          | 40 |
| 1   | 12-A  | 98/136 (72%)    | 87 (89%)   | 11 (11%)  | 6           | 6  |
| 1   | 12-B  | 94/136 (69%)    | 82 (87%)   | 12 (13%)  | 4           | 4  |
| 1   | 13-A  | 98/136 (72%)    | 80 (82%)   | 18 (18%)  | 1           | 1  |
| 1   | 13-B  | 94/136 (69%)    | 79 (84%)   | 15 (16%)  | 2           | 2  |
| 1   | 14-A  | 98/136 (72%)    | 85 (87%)   | 13 (13%)  | 4           | 4  |
| 1   | 14-B  | 94/136 (69%)    | 74 (79%)   | 20 (21%)  | 1           | 1  |
| 1   | 15-A  | 98/136 (72%)    | 86 (88%)   | 12 (12%)  | 5           | 5  |
| 1   | 15-B  | 94/136 (69%)    | 75 (80%)   | 19 (20%)  | 1           | 1  |
| 1   | 16-A  | 98/136 (72%)    | 79 (81%)   | 19 (19%)  | 1           | 1  |
| 1   | 16-B  | 94/136 (69%)    | 76 (81%)   | 18 (19%)  | 1           | 1  |
| All | All   | 3072/4352 (71%) | 2698 (88%) | 374 (12%) | 5           | 5  |

5 of 374 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 12-B  | 54  | ARG  |
| 1   | 14-B  | 24  | ARG  |
| 1   | 12-B  | 104 | VAL  |
| 1   | 13-B  | 37  | LEU  |
| 1   | 14-B  | 113 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 9-B   | 52  | GLN  |
| 1   | 16-A  | 52  | GLN  |
| 1   | 11-B  | 111 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 16-A  | 51  | HIS  |
| 1   | 14-B  | 52  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.