

# Integrative Structure Validation Report ?

February 27, 2025 - 12:15 PM PST

*The following software was used in the production of this report:*

*Integrative Modeling Validation* Version 2.0

*Python-IHM* Version 1.8

*MolProbity* Version 4.5.2

|                   |   |
|-------------------|---|
| PDB ID            | 9A13  |
| PDB-Dev ID        | PDBDEV_00000075   |
| Structure Title   | Model of the vaccinia virus DNA polymerase: complex between A20-Cter and E9 |
| Structure Authors | Bersch B; Tarbouriech N; Burmeister WP; Iseni F                             |
| Deposited on      | 2021-02-16  |

*This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.*

*We welcome your comments at [helpdesk@pdb-ihm.org](mailto:helpdesk@pdb-ihm.org)*

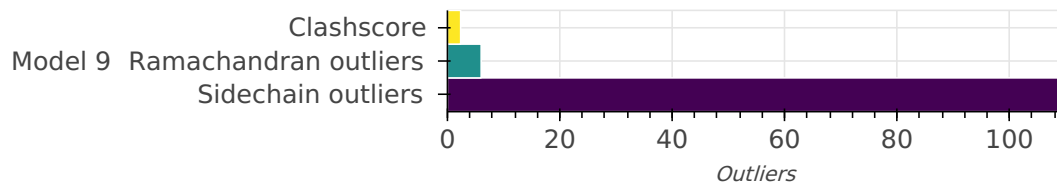
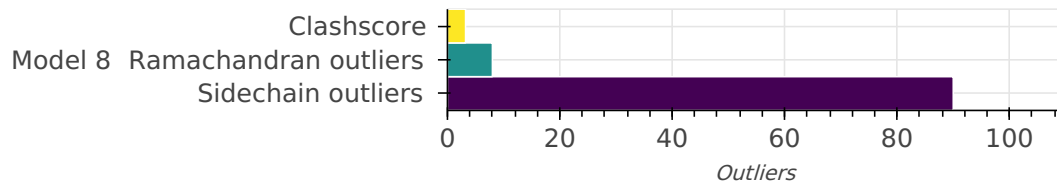
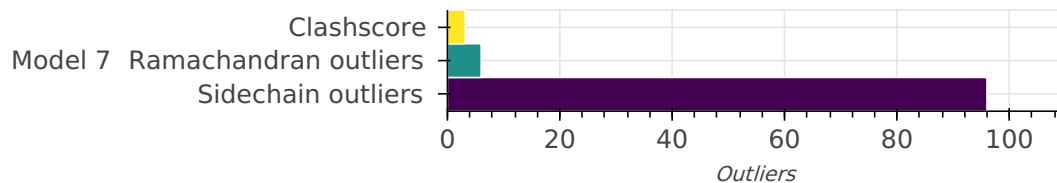
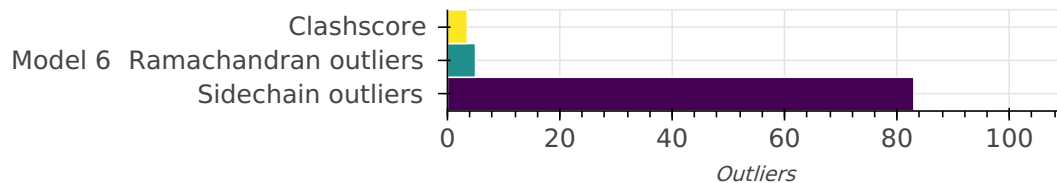
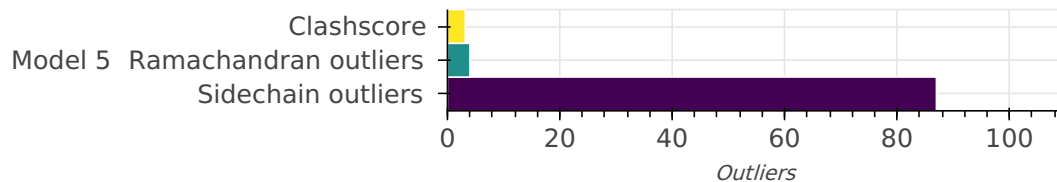
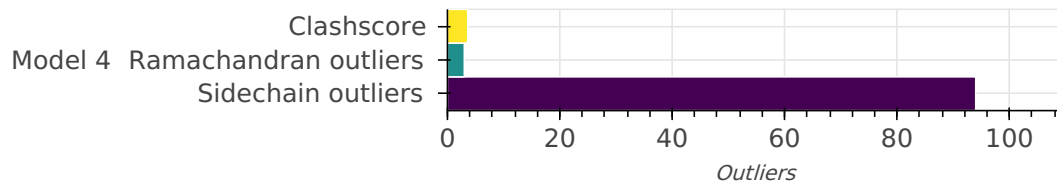
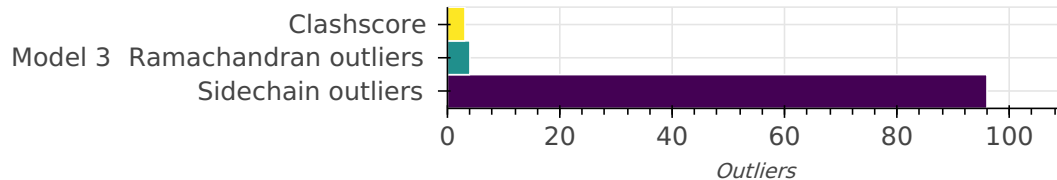
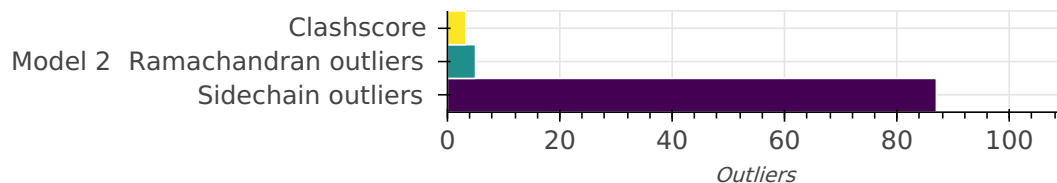
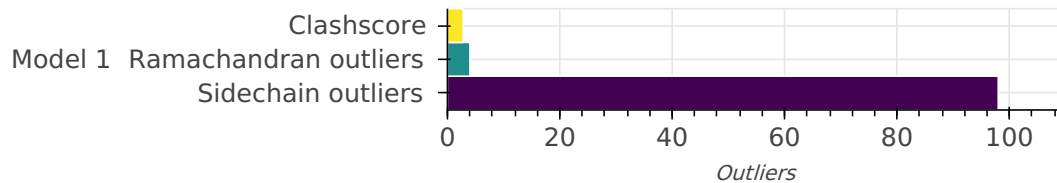
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

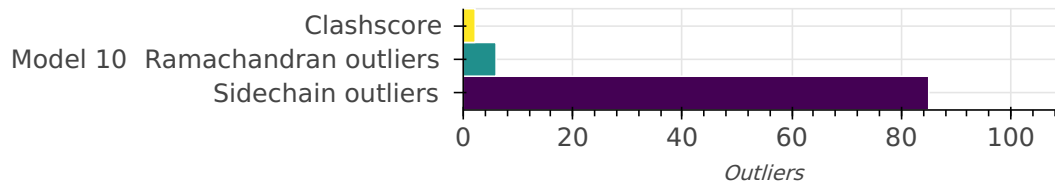
*List of references used to build this report is available [here](#).*

## Overall quality ?

*This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.*

Model Quality: MolProbity Analysis





### Ensemble information ?

*This entry consists of 0 distinct ensemble(s).*

### Summary ?

*This entry consists of 10 model(s). A total of 5 datasets were used to build this entry.*

### Representation ?

*This entry has 1 representation(s).*

| ID | Model(s) | Entity ID | Molecule name                                    | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/<br>Starting model coverage (%) | Scale  |
|----|----------|-----------|--|-----------------|----------------|----------------|-------------------|--|--------|
| 1  | 1-10     | 1         | DNA polymerase processivity factor component A20 | A               | 124            | -              | 1-124             | 100.00 / 100.00                                | Atomic |
|    |          | 2         | DNA polymerase                                   | B               | 1010           | -              | 1-1010            | 100.00 / 100.00                                | Atomic |

### Datasets used for modeling ?

*There are 5 unique datasets used to build the models in this entry.*

| ID | Dataset type       | Database name | Data access code      |
|----|--------------------|---------------|-----------------------|
| 1  | Experimental model | PDB           | <a href="#">6ZXP</a>  |
| 2  | Experimental model | PDB           | <a href="#">5N2E</a>  |
| 3  | NMR data           | BMRB          | <a href="#">34544</a> |

| ID | Dataset type | Database name | Data access code          |
|----|--------------|---------------|---------------------------|
| 4  | NMR data     | BMRB          | 34545                     |
| 5  | Other        | Not available | 10.1016/j.jmb.2021.167009 |

## Methodology and software ?

*This entry is a result of 1 distinct protocol(s).*

| Step number | Protocol ID | Method name | Method type | Method description | Number of computed models | Multi state modeling | Multi scale modeling |
|-------------|-------------|-------------|-------------|--------------------|---------------------------|----------------------|----------------------|
| 1           | 1           | None        | Docking     | None               | –                         | False                | False                |

*There is 1 software package reported in this entry.*

| ID | Software name           | Software version | Software classification | Software location   |
|----|-------------------------|------------------|-------------------------|---|
| 1  | <a href="#">HADDOCK</a> | Not available    | model building          | <a href="http://haddock.science.uu.nl/services/HADDOCK/">http://haddock.science.uu.nl/services/HADDOCK/</a> |

## Data quality ?

### NMR

Validation for this section is under development.

## Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

### Standard geometry: bond outliers ?

*There are no bond length outliers.*

### Standard geometry: angle outliers ?

*There are no bond angle outliers.*

### Too-close contacts ?

*The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all atomic models in this entry.*

| Model ID | Clash score | Number of clashes |
|----------|-------------|-------------------|
| 1        | 2.79        | 51                |
| 2        | 3.28        | 60                |

| Model ID | Clash score | Number of clashes |
|----------|-------------|-------------------|
| 3        | 3.12        | 57                |
| 4        | 3.61        | 66                |
| 5        | 3.17        | 58                |
| 6        | 3.56        | 65                |
| 7        | 3.17        | 58                |
| 8        | 3.23        | 59                |
| 9        | 2.35        | 43                |
| 10       | 2.19        | 40                |

There are 557 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom. The output is limited to 100 rows.

| Atom 1         | Atom 2         | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| B:369:VAL:HG13 | B:370:ARG:H    | 0.76     | 8                | 3              |
| B:369:VAL:HG13 | B:371:GLU:H    | 0.74     | 7                | 6              |
| B:214:GLU:HA   | B:217:ILE:HD12 | 0.71     | 10               | 1              |
| A:70:VAL:HG11  | B:582:LEU:H    | 0.69     | 7                | 1              |
| A:70:VAL:HG12  | B:581:ARG:HB3  | 0.69     | 7                | 1              |
| B:171:ILE:HG22 | B:190:THR:HG22 | 0.65     | 2                | 2              |
| B:876:LEU:HD21 | B:980:THR:HG22 | 0.65     | 7                | 1              |
| B:837:ARG:CZ   | B:837:ARG:HA   | 0.65     | 1                | 5              |
| B:128:CYS:SG   | B:159:ARG:HA   | 0.64     | 8                | 4              |
| B:904:TYR:HH   | B:908:ASP:N    | 0.63     | 4                | 2              |
| B:502:ALA:HA   | B:505:VAL:HG22 | 0.63     | 7                | 8              |
| B:390:ALA:HB1  | B:414:ILE:HG23 | 0.62     | 5                | 5              |
| B:220:ALA:HB2  | B:453:LEU:HD11 | 0.60     | 5                | 2              |
| B:724:ASN:HB3  | B:727:TYR:O    | 0.59     | 7                | 5              |
| B:182:VAL:HG11 | B:278:ASN:HB3  | 0.59     | 2                | 3              |
| B:685:TYR:CZ   | B:689:LYS:HD2  | 0.59     | 5                | 7              |
| B:711:LEU:O    | B:746:ARG:HA   | 0.58     | 6                | 6              |
| B:269:HIS:HA   | B:273:LEU:HD12 | 0.58     | 1                | 1              |
| B:580:ASN:OD1  | B:582:LEU:HB3  | 0.58     | 7                | 2              |
| B:125:PRO:HB2  | B:487:ALA:HB1  | 0.57     | 6                | 2              |
| B:309:SER:HA   | B:318:ALA:N    | 0.57     | 3                | 2              |
| A:77:ILE:HD12  | B:586:ILE:HG12 | 0.57     | 1                | 3              |
| A:114:VAL:O    | A:118:VAL:HG23 | 0.57     | 8                | 1              |
| B:80:LEU:HD22  | B:590:LEU:HB3  | 0.57     | 3                | 1              |

| Atom 1         | Atom 2         | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| B:165:SER:O    | B:261:ASP:HB2  | 0.57     | 8                | 4              |
| A:6:PHE:O      | A:12:ALA:HA    | 0.57     | 9                | 1              |
| B:892:GLU:HA   | B:895:MET:SD   | 0.56     | 6                | 5              |
| B:836:ARG:HA   | B:836:ARG:NE   | 0.56     | 8                | 1              |
| B:587:ASN:O    | B:591:LEU:HG   | 0.56     | 5                | 4              |
| B:900:HIS:ND1  | B:928:LEU:HA   | 0.56     | 4                | 2              |
| B:774:ILE:O    | B:778:LEU:HG   | 0.56     | 3                | 1              |
| B:27:ARG:NH2   | B:164:ARG:HA   | 0.55     | 3                | 3              |
| B:909:ASN:N    | B:910:PRO:HD2  | 0.55     | 5                | 8              |
| B:221:VAL:HA   | B:225:CYS:O    | 0.55     | 2                | 6              |
| A:50:SER:OG    | A:53:ASP:HB2   | 0.55     | 6                | 1              |
| A:42:VAL:O     | A:46:ILE:HG12  | 0.54     | 2                | 8              |
| B:72:ILE:HD13  | B:521:LEU:HB3  | 0.54     | 3                | 2              |
| B:409:VAL:HG11 | B:412:LYS:HD3  | 0.54     | 10               | 2              |
| A:63:GLU:O     | A:67:ILE:HG13  | 0.54     | 5                | 5              |
| B:359:SER:O    | B:385:LYS:HE3  | 0.54     | 9                | 1              |
| A:8:LYS:O      | A:9:VAL:HG22   | 0.53     | 4                | 1              |
| B:541:LYS:HB2  | B:752:VAL:HG13 | 0.53     | 7                | 1              |
| B:453:LEU:O    | B:457:LEU:HG   | 0.53     | 9                | 1              |
| B:627:ILE:HB   | B:628:PRO:HD3  | 0.53     | 5                | 10             |
| B:171:ILE:HG22 | B:190:THR:HG23 | 0.53     | 10               | 2              |
| B:71:ASP:HA    | B:522:VAL:O    | 0.53     | 6                | 1              |
| B:409:VAL:HG13 | B:421:VAL:HG21 | 0.53     | 7                | 1              |
| B:843:HIS:CE1  | B:979:LEU:HA   | 0.53     | 2                | 3              |
| B:126:ASP:HB3  | B:487:ALA:HB3  | 0.53     | 6                | 1              |
| B:25:LYS:NZ    | B:261:ASP:HA   | 0.53     | 4                | 2              |
| B:112:LEU:HD13 | B:492:LEU:HD21 | 0.53     | 9                | 1              |
| B:837:ARG:HA   | B:837:ARG:NH1  | 0.52     | 1                | 1              |
| B:468:CYS:O    | B:471:GLN:HG2  | 0.52     | 3                | 4              |
| B:559:PRO:HA   | B:631:LEU:HD13 | 0.52     | 5                | 1              |
| B:582:LEU:O    | B:586:ILE:HG13 | 0.52     | 6                | 1              |
| B:444:LEU:HD22 | B:459:MET:HE3  | 0.52     | 6                | 1              |
| B:490:TYR:CG   | B:505:VAL:HB   | 0.52     | 1                | 1              |
| B:264:VAL:HA   | B:333:PHE:O    | 0.52     | 5                | 5              |
| B:443:ASP:O    | B:447:MET:HB2  | 0.52     | 7                | 2              |

| Atom 1         | Atom 2         | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| B:482:LYS:HE2  | B:662:TYR:CD2  | 0.52     | 10               | 3              |
| B:581:ARG:HD3  | B:584:GLU:OE1  | 0.52     | 3                | 1              |
| B:12:TRP:CE2   | B:24:LEU:HD13  | 0.52     | 8                | 3              |
| B:586:ILE:O    | B:590:LEU:HB2  | 0.52     | 6                | 1              |
| B:6:ASP:O      | B:28:CYS:HA    | 0.51     | 9                | 1              |
| B:834:GLU:HA   | B:838:ASP:HB3  | 0.51     | 9                | 1              |
| B:404:ASP:OD2  | B:835:THR:HB   | 0.51     | 1                | 1              |
| B:939:PRO:HB2  | B:941:ASN:OD1  | 0.51     | 3                | 1              |
| A:17:LEU:HD21  | A:111:ILE:HG23 | 0.51     | 4                | 1              |
| B:274:ARG:NH2  | B:303:ILE:HB   | 0.51     | 3                | 1              |
| B:556:SER:O    | B:560:ASN:HB2  | 0.51     | 4                | 2              |
| B:631:LEU:HD21 | B:671:VAL:HG21 | 0.51     | 4                | 1              |
| B:368:GLY:O    | B:369:VAL:HG12 | 0.50     | 5                | 5              |
| B:336:TYR:O    | B:340:GLN:HB2  | 0.50     | 3                | 1              |
| B:11:ASN:HB3   | B:25:LYS:HB3   | 0.50     | 4                | 5              |
| A:72:ASN:HB2   | A:92:CYS:SG    | 0.50     | 10               | 2              |
| B:858:LEU:HA   | B:863:MET:SD   | 0.50     | 8                | 2              |
| B:266:PHE:O    | B:267:ASN:HB3  | 0.50     | 5                | 2              |
| B:254:GLN:O    | B:258:LEU:HG   | 0.50     | 1                | 4              |
| B:876:LEU:O    | B:880:LEU:HG   | 0.50     | 10               | 3              |
| B:852:THR:O    | B:856:GLU:HG3  | 0.50     | 1                | 2              |
| B:77:SER:O     | B:576:VAL:HA   | 0.50     | 3                | 2              |
| B:672:TYR:HA   | B:675:MET:SD   | 0.50     | 5                | 1              |
| B:791:PHE:C    | B:792:LYS:HG2  | 0.49     | 2                | 2              |
| B:724:ASN:HB2  | B:729:ASP:OD2  | 0.49     | 3                | 1              |
| B:866:ASN:O    | B:870:ILE:HG12 | 0.49     | 2                | 1              |
| B:869:CYS:SG   | B:992:LEU:HD23 | 0.49     | 10               | 3              |
| B:110:GLU:O    | B:507:LYS:HD3  | 0.49     | 10               | 1              |
| A:80:CYS:SG    | B:590:LEU:HD21 | 0.49     | 9                | 1              |
| B:402:ASP:HB3  | B:405:ILE:HD13 | 0.49     | 2                | 1              |
| B:349:LYS:HB3  | B:351:ASP:OD1  | 0.49     | 3                | 2              |
| B:837:ARG:HD3  | B:895:MET:O    | 0.49     | 5                | 1              |
| B:209:GLU:HG2  | B:217:ILE:HD13 | 0.49     | 2                | 1              |
| B:78:TYR:HA    | B:577:VAL:O    | 0.49     | 6                | 3              |
| A:62:PRO:O     | A:66:PHE:HB2   | 0.49     | 10               | 2              |

| Atom 1         | Atom 2         | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| B:121:ASN:ND2  | B:149:PRO:HG2  | 0.49     | 8                | 2              |
| B:579:THR:HG23 | B:612:LEU:HD23 | 0.49     | 2                | 2              |
| B:981:SER:O    | B:985:ASN:HB2  | 0.48     | 4                | 1              |
| B:59:PHE:HB2   | B:98:PRO:HD3   | 0.48     | 2                | 1              |
| B:48:ASP:O     | B:52:GLN:HG2   | 0.48     | 4                | 3              |
| B:670:SER:O    | B:674:LEU:HG   | 0.48     | 4                | 2              |

### Torsion angles: Protein backbone ?

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

| Model ID | Analysed | Favored | Allowed | Outliers |
|----------|----------|---------|---------|----------|
| 1        | 1115     | 1048    | 63      | 4        |
| 2        | 1115     | 1046    | 64      | 5        |
| 3        | 1115     | 1048    | 63      | 4        |
| 4        | 1115     | 1040    | 72      | 3        |
| 5        | 1115     | 1040    | 71      | 4        |
| 6        | 1115     | 1050    | 60      | 5        |
| 7        | 1115     | 1054    | 55      | 6        |
| 8        | 1115     | 1045    | 62      | 8        |
| 9        | 1115     | 1048    | 61      | 6        |
| 10       | 1115     | 1049    | 60      | 6        |

There are 19 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A     | 9   | VAL  | 9              |
| B     | 369 | VAL  | 9              |
| B     | 184 | ILE  | 4              |
| B     | 835 | THR  | 4              |
| B     | 949 | VAL  | 4              |
| B     | 834 | GLU  | 3              |
| A     | 7   | SER  | 2              |
| B     | 531 | PRO  | 2              |
| B     | 532 | TYR  | 2              |
| B     | 713 | ASN  | 2              |
| B     | 943 | PRO  | 2              |
| A     | 4   | LYS  | 1              |



| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| B     | 79  | ASN  | 1              |
| B     | 177 | LYS  | 1              |
| B     | 272 | ASP  | 1              |
| B     | 404 | ASP  | 1              |
| B     | 500 | TYR  | 1              |
| B     | 789 | ASN  | 1              |
| B     | 887 | ARG  | 1              |

### Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

| Model ID | Analysed | Favored | Allowed | Outliers |
|----------|----------|---------|---------|----------|
| 1        | 1036     | 834     | 104     | 98       |
| 2        | 1036     | 838     | 111     | 87       |
| 3        | 1036     | 839     | 101     | 96       |
| 4        | 1036     | 843     | 99      | 94       |
| 5        | 1036     | 834     | 115     | 87       |
| 6        | 1036     | 838     | 115     | 83       |
| 7        | 1036     | 829     | 111     | 96       |
| 8        | 1036     | 826     | 120     | 90       |
| 9        | 1036     | 807     | 120     | 109      |
| 10       | 1036     | 831     | 120     | 85       |

There are 333 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A     | 90  | THR  | 10             |
| B     | 15  | SER  | 10             |
| B     | 495 | SER  | 10             |
| B     | 526 | THR  | 10             |
| B     | 530 | PHE  | 10             |
| B     | 568 | SER  | 10             |
| B     | 169 | LEU  | 9              |
| B     | 244 | SER  | 9              |
| B     | 308 | GLN  | 9              |
| B     | 602 | THR  | 9              |

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| B     | 740 | SER  | 9              |
| B     | 834 | GLU  | 9              |
| A     | 11  | SER  | 8              |
| A     | 41  | THR  | 8              |
| B     | 55  | SER  | 8              |
| B     | 213 | THR  | 8              |
| B     | 481 | THR  | 8              |
| B     | 503 | SER  | 8              |
| B     | 953 | THR  | 8              |
| B     | 961 | SER  | 8              |
| A     | 32  | LEU  | 7              |
| B     | 219 | GLU  | 7              |
| B     | 259 | THR  | 7              |
| B     | 296 | LYS  | 7              |
| B     | 309 | SER  | 7              |
| B     | 407 | CYS  | 7              |
| B     | 504 | THR  | 7              |
| B     | 712 | SER  | 7              |
| B     | 821 | SER  | 7              |
| B     | 840 | SER  | 7              |
| B     | 925 | THR  | 7              |
| A     | 17  | LEU  | 6              |
| A     | 50  | SER  | 6              |
| B     | 281 | GLU  | 6              |
| B     | 284 | THR  | 6              |
| B     | 321 | THR  | 6              |
| B     | 361 | MET  | 6              |
| B     | 369 | VAL  | 6              |
| B     | 652 | THR  | 6              |
| B     | 816 | SER  | 6              |
| B     | 818 | SER  | 6              |
| B     | 832 | THR  | 6              |
| B     | 888 | SER  | 6              |
| B     | 16  | HIS  | 5              |
| B     | 73  | ASP  | 5              |

| Chain | Res  | Type | Models (Total) |
|-------|------|------|----------------|
| B     | 91   | ASP  | 5              |
| B     | 190  | THR  | 5              |
| B     | 222  | ASP  | 5              |
| B     | 265  | THR  | 5              |
| B     | 310  | SER  | 5              |
| B     | 377  | ASP  | 5              |
| B     | 614  | SER  | 5              |
| B     | 670  | SER  | 5              |
| B     | 704  | SER  | 5              |
| B     | 723  | SER  | 5              |
| B     | 739  | THR  | 5              |
| B     | 755  | ASP  | 5              |
| B     | 761  | THR  | 5              |
| B     | 833  | SER  | 5              |
| B     | 1004 | LYS  | 5              |
| A     | 8    | LYS  | 4              |
| A     | 28   | THR  | 4              |
| A     | 66   | PHE  | 4              |
| A     | 74   | ARG  | 4              |
| A     | 113  | ASN  | 4              |
| A     | 117  | ASP  | 4              |
| B     | 14   | GLU  | 4              |
| B     | 27   | ARG  | 4              |
| B     | 69   | THR  | 4              |
| B     | 104  | GLN  | 4              |
| B     | 137  | THR  | 4              |
| B     | 176  | ASP  | 4              |
| B     | 177  | LYS  | 4              |
| B     | 231  | LEU  | 4              |
| B     | 413  | ASP  | 4              |
| B     | 428  | LEU  | 4              |
| B     | 484  | ASP  | 4              |
| B     | 525  | GLU  | 4              |
| B     | 579  | THR  | 4              |
| B     | 637  | GLU  | 4              |

| Chain | Res  | Type | Models (Total) |
|-------|------|------|----------------|
| B     | 651  | SER  | 4              |
| B     | 751  | SER  | 4              |
| B     | 756  | THR  | 4              |
| B     | 819  | SER  | 4              |
| B     | 855  | SER  | 4              |
| B     | 862  | ARG  | 4              |
| B     | 873  | LEU  | 4              |
| B     | 945  | THR  | 4              |
| B     | 959  | ASP  | 4              |
| B     | 971  | PHE  | 4              |
| B     | 997  | PHE  | 4              |
| B     | 1003 | SER  | 4              |
| B     | 1006 | THR  | 4              |
| A     | 59   | LEU  | 3              |
| A     | 75   | PHE  | 3              |
| A     | 97   | SER  | 3              |
| A     | 119  | LYS  | 3              |
| B     | 26   | SER  | 3              |
| B     | 53   | SER  | 3              |
| B     | 71   | ASP  | 3              |

### Fit of model to data used for modeling ?

#### NMR

Validation for this section is under development.

### Fit of model to data used for validation ?

Validation for this section is under development.

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