# Integrative Structure Validation Report

## October 09, 2025 - 04:40 PM PDT

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

*IHMValidation Version 3.0*
*Python-IHM Version 2.5*
*MolProbity Version 4.5.2*
*ATSAS Version 3.2.1 (r14885)*

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| | |
|---|---|
| PDB ID | 9A1V \| pdb_00009a1v |
| PDB-Dev ID | PDBDEV_00000124 |
| Structure Title | Integrative model of Nucleotide excision repair complex of XPA and RPA on 5' junction substrate |
| Structure Authors | DSouza, A.; Topolska-Wos, A.M.; Chazin, W.J. |
| Deposited on | 2022-06-03 |

*This is a PDB-IHM Structure Validation Report.*

*We welcome your comments at helpdesk@pdb-ihm.org*

*A user guide is available at 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.*

# 1. Overview

## 1.1. Summary

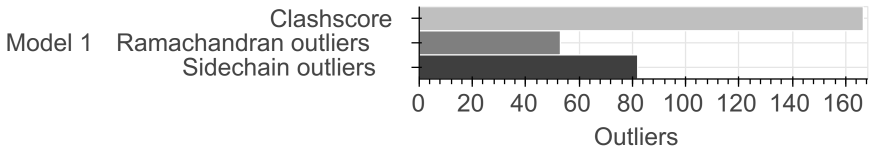
*This entry consists of 1 model(s). A total of 7 dataset(s) were used to build this entry.*

| Name | Type | Count |
|---|---|---|
| SAS data | Experimental data | 1 |
| Experimental model | Starting model | 3 |
| Comparative model | Starting model | 1 |
| Integrative model | Starting model | 1 |
| De Novo model | Starting model | 1 |

## 1.2. 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



## 2. Model Details

### 2.1. Ensemble information

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

### 2.2. 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/ Starting model coverage (%) | Scale |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | RPA70 | A | 434 | - | 1-238, 239-253, 254-434 | 100.00 / 100.00 | Atomic |
| | | 2 | RPA32 | B | 226 | - | 1-128, 129-226 | 100.00 / 100.00 | Atomic |
| | | 3 | RPA14 | C | 115 | - | 1-115 | 100.00 / 100.00 | Atomic |
| | | 4 | XPA | D | 239 | - | 1-28, 29-48, 49-97, 98-239 | 100.00 / 100.00 | Atomic |
| | | 5 | DNA (5'-D(P*GP*GP*CP*CP*CP*GP*CP*GP*GP*CP*TP*TP*TP*TP*TP*TP*TP*T)-3') | E | 18 | - | 1-18 | 100.00 / 100.00 | Atomic |
| | | 6 | DNA (40-MER) | F | 40 | - | 1-40 | 100.00 / 100.00 | Atomic |
| | | 7 | ZINC ION | G<br>H | Non-polymeric | - | - | Not available / Not available | Atomic |

### 2.3. Datasets used for modeling

*There are 7 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 1 | SAS data | SASBDB | SASDP24 |
| 2 | Experimental model | PDB | pdb_00001jmc |
| 3 | Integrative model | PDB | pdb_00009a03 |
| 4 | Experimental model | PDB | pdb_00001l1o |
| 5 | Experimental model | PDB | pdb_00001dpu |
| 6 | Comparative model | Not available | Not available |
| 7 | De Novo model | Not available | Not available |

## 2.4. 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 | Not available | Not available | Not available | 1 | False | False |

*There are 2 software packages reported in this entry.*

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 1 | Modeller | 9v4 | model building | https://salilab.org/modeller/ |
| 2 | FoXSDock | main.c2a7893 | model building | https://modbase.compbio.ucsf.edu/foxsdock/ |

# 3. Data quality ?

### 3.1.1. Scattering profile

SAS data used in this integrative model could not be validated as the sasCIF file is currently unavailable or incomplete.

# 4. 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.

## 4.1b. MolProbity Analysis ?

*Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-partice or particle-atom pairs for which excluded volume was analysed.*

### Standard geometry: bond outliers ?

*There are 150 bond length outliers in this entry (1.59% of 9422 assessed bonds). A summary is provided below. The output is limited to 100 rows.*

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| F | 27 | DC | O3'-P | 33.50 | 2.11 | 1.61 | 1 | 1 |
| B | 156 | MET | C-N | 26.94 | 1.77 | 1.34 | 1 | 1 |
| B | 155 | PHE | CA-C | 26.47 | 2.08 | 1.52 | 1 | 1 |
| B | 157 | PRO | C-N | 25.85 | 1.69 | 1.33 | 1 | 1 |
| B | 157 | PRO | N-CA | 24.22 | 1.83 | 1.47 | 1 | 1 |
| B | 155 | PHE | C-N | 23.60 | 1.66 | 1.33 | 1 | 1 |
| B | 157 | PRO | CA-C | 21.60 | 1.98 | 1.52 | 1 | 1 |
| B | 154 | SER | C-N | 21.14 | 1.63 | 1.33 | 1 | 1 |
| B | 156 | MET | CA-C | 20.38 | 1.95 | 1.52 | 1 | 1 |
| F | 21 | DC | O3'-P | 19.91 | 1.91 | 1.61 | 1 | 1 |
| F | 25 | DC | P-O5' | 19.72 | 1.99 | 1.60 | 1 | 1 |
| F | 27 | DC | C3'-C2' | 18.59 | 1.90 | 1.52 | 1 | 1 |
| B | 156 | MET | N-CA | 18.07 | 1.80 | 1.46 | 1 | 1 |
| F | 22 | DC | O3'-P | 16.63 | 1.86 | 1.61 | 1 | 1 |
| F | 24 | DC | P-O5' | 16.48 | 1.93 | 1.60 | 1 | 1 |
| F | 24 | DC | C5'-C4' | 14.52 | 1.81 | 1.52 | 1 | 1 |
| F | 27 | DC | C5'-C4' | 13.36 | 1.25 | 1.52 | 1 | 1 |
| B | 155 | PHE | N-CA | 12.39 | 1.69 | 1.46 | 1 | 1 |
| F | 27 | DC | C3'-O3' | 12.38 | 1.79 | 1.42 | 1 | 1 |
| B | 153 | ASN | C-N | 12.01 | 1.50 | 1.33 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| D | 61 | ASN | C-N | 11.99 | 1.50 | 1.33 | 1 | 1 |
| B | 152 | GLY | C-N | 11.95 | 1.50 | 1.33 | 1 | 1 |
| B | 151 | GLY | C-N | 10.88 | 1.48 | 1.33 | 1 | 1 |
| B | 147 | ALA | C-N | 10.83 | 1.48 | 1.33 | 1 | 1 |
| B | 136 | ARG | C-N | 10.83 | 1.48 | 1.33 | 1 | 1 |
| F | 23 | DC | O3'-P | 10.80 | 1.77 | 1.61 | 1 | 1 |
| B | 133 | SER | C-N | 10.75 | 1.48 | 1.33 | 1 | 1 |
| B | 150 | PHE | C-N | 10.75 | 1.48 | 1.33 | 1 | 1 |
| B | 140 | SER | C-N | 10.74 | 1.48 | 1.33 | 1 | 1 |
| B | 142 | PRO | C-N | 10.72 | 1.48 | 1.33 | 1 | 1 |
| B | 138 | PRO | C-N | 10.68 | 1.48 | 1.33 | 1 | 1 |
| B | 144 | MET | C-N | 10.63 | 1.48 | 1.33 | 1 | 1 |
| B | 143 | GLY | C-N | 10.63 | 1.48 | 1.33 | 1 | 1 |
| B | 149 | ASN | C-N | 10.63 | 1.48 | 1.33 | 1 | 1 |
| B | 139 | ILE | C-N | 10.61 | 1.48 | 1.33 | 1 | 1 |
| B | 145 | SER | C-N | 10.51 | 1.48 | 1.33 | 1 | 1 |
| B | 146 | GLU | C-N | 10.50 | 1.48 | 1.33 | 1 | 1 |
| B | 135 | GLY | C-N | 10.42 | 1.47 | 1.33 | 1 | 1 |
| B | 134 | ALA | C-N | 10.32 | 1.47 | 1.33 | 1 | 1 |
| B | 154 | SER | CA-C | 10.11 | 1.74 | 1.52 | 1 | 1 |
| B | 148 | GLY | C-N | 9.86 | 1.47 | 1.33 | 1 | 1 |
| B | 132 | PRO | C-N | 9.85 | 1.47 | 1.33 | 1 | 1 |
| F | 22 | DC | P-O5' | 9.82 | 1.80 | 1.60 | 1 | 1 |
| B | 135 | GLY | CA-C | 9.81 | 1.69 | 1.52 | 1 | 1 |
| D | 62 | VAL | N-CA | 9.81 | 1.64 | 1.46 | 1 | 1 |
| F | 25 | DC | O5'-C5' | 9.71 | 1.71 | 1.42 | 1 | 1 |
| F | 25 | DC | C5'-C4' | 9.48 | 1.71 | 1.52 | 1 | 1 |
| B | 130 | SER | C-N | 9.29 | 1.46 | 1.33 | 1 | 1 |
| F | 26 | DC | O3'-P | 9.23 | 1.47 | 1.61 | 1 | 1 |
| B | 129 | ASN | C-N | 9.09 | 1.46 | 1.33 | 1 | 1 |
| B | 138 | PRO | N-CA | 9.07 | 1.60 | 1.47 | 1 | 1 |
| B | 152 | GLY | CA-C | 9.05 | 1.68 | 1.52 | 1 | 1 |
| B | 151 | GLY | CA-C | 8.96 | 1.68 | 1.52 | 1 | 1 |
| B | 142 | PRO | N-CA | 8.95 | 1.60 | 1.47 | 1 | 1 |
| B | 143 | GLY | CA-C | 8.85 | 1.68 | 1.52 | 1 | 1 |
| B | 148 | GLY | CA-C | 8.85 | 1.68 | 1.52 | 1 | 1 |
| B | 128 | LYS | C-N | 8.84 | 1.45 | 1.33 | 1 | 1 |
| F | 23 | DC | C4-C5 | 8.66 | 1.25 | 1.43 | 1 | 1 |
| B | 152 | GLY | N-CA | 8.57 | 1.59 | 1.45 | 1 | 1 |
| B | 137 | ALA | C-N | 8.56 | 1.48 | 1.34 | 1 | 1 |
| B | 141 | ASN | C-N | 8.53 | 1.48 | 1.34 | 1 | 1 |
| B | 135 | GLY | N-CA | 8.38 | 1.59 | 1.45 | 1 | 1 |
| B | 151 | GLY | N-CA | 8.35 | 1.58 | 1.45 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| B | 143 | GLY | N-CA | 8.20 | 1.58 | 1.45 | 1 | 1 |
| F | 28 | DC | P-OP2 | 8.17 | 1.32 | 1.48 | 1 | 1 |
| B | 153 | ASN | CA-C | 8.08 | 1.69 | 1.52 | 1 | 1 |
| D | 62 | VAL | CA-C | 7.91 | 1.69 | 1.52 | 1 | 1 |
| F | 24 | DC | O5'-C5' | 7.88 | 1.66 | 1.42 | 1 | 1 |
| F | 22 | DC | O4'-C1' | 7.79 | 1.26 | 1.41 | 1 | 1 |
| B | 154 | SER | N-CA | 7.78 | 1.61 | 1.46 | 1 | 1 |
| B | 133 | SER | CA-C | 7.78 | 1.69 | 1.52 | 1 | 1 |
| F | 28 | DC | P-OP1 | 7.75 | 1.32 | 1.48 | 1 | 1 |
| B | 134 | ALA | CA-C | 7.66 | 1.69 | 1.52 | 1 | 1 |
| B | 148 | GLY | N-CA | 7.65 | 1.57 | 1.45 | 1 | 1 |
| F | 24 | DC | C1'-N1 | 7.65 | 1.72 | 1.49 | 1 | 1 |
| B | 137 | ALA | CA-C | 7.55 | 1.68 | 1.52 | 1 | 1 |
| B | 141 | ASN | CA-C | 7.55 | 1.68 | 1.52 | 1 | 1 |
| F | 28 | DC | P-O5' | 7.35 | 1.75 | 1.60 | 1 | 1 |
| B | 153 | ASN | N-CA | 7.35 | 1.60 | 1.46 | 1 | 1 |
| B | 147 | ALA | CA-C | 7.33 | 1.68 | 1.52 | 1 | 1 |
| B | 140 | SER | CA-C | 7.32 | 1.68 | 1.52 | 1 | 1 |
| F | 26 | DC | C2'-C1' | 7.29 | 1.38 | 1.52 | 1 | 1 |
| B | 155 | PHE | CA-CB | 7.26 | 1.68 | 1.53 | 1 | 1 |
| B | 132 | PRO | N-CA | 7.14 | 1.57 | 1.47 | 1 | 1 |
| B | 139 | ILE | CA-C | 7.13 | 1.67 | 1.52 | 1 | 1 |
| B | 134 | ALA | N-CA | 7.12 | 1.59 | 1.46 | 1 | 1 |
| F | 23 | DC | C4'-C3' | 7.09 | 1.66 | 1.52 | 1 | 1 |
| B | 150 | PHE | CA-C | 7.06 | 1.67 | 1.52 | 1 | 1 |
| B | 136 | ARG | CA-C | 7.05 | 1.67 | 1.52 | 1 | 1 |
| B | 145 | SER | CA-C | 7.02 | 1.67 | 1.52 | 1 | 1 |
| B | 138 | PRO | CA-C | 7.01 | 1.67 | 1.52 | 1 | 1 |
| B | 142 | PRO | CA-C | 6.96 | 1.67 | 1.52 | 1 | 1 |
| F | 22 | DC | N1-C2 | 6.96 | 1.26 | 1.40 | 1 | 1 |
| B | 146 | GLU | CA-C | 6.94 | 1.67 | 1.52 | 1 | 1 |
| B | 144 | MET | CA-C | 6.93 | 1.67 | 1.52 | 1 | 1 |
| B | 131 | GLN | C-N | 6.86 | 1.45 | 1.34 | 1 | 1 |
| F | 23 | DC | P-O5' | 6.81 | 1.74 | 1.60 | 1 | 1 |
| B | 149 | ASN | N-CA | 6.76 | 1.59 | 1.46 | 1 | 1 |
| F | 22 | DC | C3'-O3' | 6.74 | 1.62 | 1.42 | 1 | 1 |
| F | 27 | DC | C2'-C1' | 6.69 | 1.39 | 1.52 | 1 | 1 |

## Standard geometry: angle outliers ?

*There are 505 bond angle outliers in this entry (3.90% of 12943 assessed bonds). A summary is provided below. The output is limited to 100 rows.*

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| F | 21 | DC | P-O5'-C5' | 36.33 | 65.50 | 120.00 | 1 | 1 |
| F | 27 | DC | C3'-O3'-P | 33.94 | 171.11 | 120.20 | 1 | 1 |
| F | 26 | DC | C3'-O3'-P | 33.78 | 69.52 | 120.20 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| F | 25 | DC | P-O5'-C5' | 29.92 | 164.88 | 120.00 | 1 | 1 |
| F | 21 | DC | O3'-P-O5' | 28.37 | 146.56 | 104.00 | 1 | 1 |
| F | 24 | DC | P-O5'-C5' | 24.97 | 157.46 | 120.00 | 1 | 1 |
| F | 27 | DC | O3'-P-O5' | 24.80 | 141.20 | 104.00 | 1 | 1 |
| F | 22 | DC | P-O5'-C5' | 24.45 | 156.68 | 120.00 | 1 | 1 |
| F | 21 | DC | C3'-O3'-P | 21.57 | 152.55 | 120.20 | 1 | 1 |
| F | 22 | DC | OP1-P-O5' | 20.71 | 46.86 | 109.00 | 1 | 1 |
| F | 27 | DC | C4'-C3'-O3' | 20.08 | 140.12 | 110.00 | 1 | 1 |
| F | 22 | DC | C2'-C1'-N1 | 18.11 | 140.67 | 113.50 | 1 | 1 |
| B | 157 | PRO | N-CA-C | 17.96 | 156.99 | 112.10 | 1 | 1 |
| F | 23 | DC | P-O5'-C5' | 17.87 | 146.80 | 120.00 | 1 | 1 |
| F | 23 | DC | C4'-C3'-O3' | 17.26 | 135.88 | 110.00 | 1 | 1 |
| F | 23 | DC | C3'-O3'-P | 17.25 | 146.08 | 120.20 | 1 | 1 |
| F | 22 | DC | C3'-O3'-P | 17.13 | 145.89 | 120.20 | 1 | 1 |
| F | 28 | DC | O5'-C5'-C4' | 16.53 | 135.59 | 110.80 | 1 | 1 |
| F | 27 | DC | C5'-C4'-O4' | 16.51 | 84.64 | 109.40 | 1 | 1 |
| B | 157 | PRO | CA-C-N | 16.36 | 148.91 | 116.20 | 1 | 1 |
| F | 28 | DC | P-O5'-C5' | 16.10 | 144.15 | 120.00 | 1 | 1 |
| B | 156 | MET | CA-C-N | 15.02 | 139.43 | 116.90 | 1 | 1 |
| F | 22 | DC | C4'-C3'-C2' | 15.01 | 79.89 | 102.40 | 1 | 1 |
| B | 154 | SER | C-N-CA | 14.77 | 148.28 | 121.70 | 1 | 1 |
| F | 11 | DC | O3'-P-OP1 | 14.49 | 64.52 | 108.00 | 1 | 1 |
| D | 61 | ASN | C-N-CA | 14.36 | 147.56 | 121.70 | 1 | 1 |
| F | 21 | DC | C4'-C3'-O3' | 14.29 | 131.44 | 110.00 | 1 | 1 |
| F | 24 | DC | C2-N1-C6 | 14.24 | 99.24 | 120.60 | 1 | 1 |
| F | 26 | DC | O4'-C1'-N1 | 14.23 | 129.74 | 108.40 | 1 | 1 |
| F | 23 | DC | O3'-P-O5' | 14.21 | 125.31 | 104.00 | 1 | 1 |
| F | 11 | DC | O3'-P-OP2 | 14.11 | 65.67 | 108.00 | 1 | 1 |
| F | 24 | DC | C4'-C3'-O3' | 14.07 | 131.11 | 110.00 | 1 | 1 |
| D | 51 | THR | C-CA-CB | 14.06 | 140.02 | 109.10 | 1 | 1 |
| F | 24 | DC | C5'-C4'-C3' | 13.76 | 135.54 | 114.90 | 1 | 1 |
| F | 23 | DC | O4'-C1'-N1 | 13.64 | 128.86 | 108.40 | 1 | 1 |
| F | 26 | DC | C2'-C1'-N1 | 13.56 | 133.84 | 113.50 | 1 | 1 |
| F | 21 | DC | C3'-C2'-C1' | 13.41 | 121.71 | 101.60 | 1 | 1 |
| F | 27 | DC | C2'-C1'-N1 | 13.30 | 133.45 | 113.50 | 1 | 1 |
| F | 22 | DC | O3'-C3'-C2' | 13.28 | 131.43 | 111.50 | 1 | 1 |
| F | 24 | DC | O3'-P-O5' | 13.12 | 123.68 | 104.00 | 1 | 1 |
| D | 133 | ASP | C-N-CA | 13.10 | 145.29 | 121.70 | 1 | 1 |
| B | 148 | GLY | C-N-CA | 13.09 | 145.26 | 121.70 | 1 | 1 |
| B | 154 | SER | CA-C-N | 12.96 | 142.12 | 116.20 | 1 | 1 |
| D | 134 | ASP | C-N-CA | 12.85 | 144.83 | 121.70 | 1 | 1 |
| F | 22 | DC | O3'-P-O5' | 12.73 | 123.10 | 104.00 | 1 | 1 |
| B | 153 | ASN | C-N-CA | 12.60 | 144.38 | 121.70 | 1 | 1 |
| F | 28 | DC | C4'-C3'-O3' | 12.52 | 128.77 | 110.00 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| B | 155 | PHE | C-N-CA | 12.48 | 144.17 | 121.70 | 1 | 1 |
| F | 22 | DC | C4'-C3'-O3' | 12.42 | 128.63 | 110.00 | 1 | 1 |
| F | 24 | DC | O5'-C5'-C4' | 12.00 | 128.80 | 110.80 | 1 | 1 |
| F | 22 | DC | C5'-C4'-C3' | 11.90 | 132.75 | 114.90 | 1 | 1 |
| F | 22 | DC | C2-N1-C6 | 11.81 | 102.88 | 120.60 | 1 | 1 |
| F | 27 | DC | O3'-C3'-C2' | 11.63 | 128.95 | 111.50 | 1 | 1 |
| F | 24 | DC | C2'-C1'-N1 | 11.62 | 130.93 | 113.50 | 1 | 1 |
| B | 154 | SER | CA-C-O | 11.51 | 101.23 | 120.80 | 1 | 1 |
| F | 25 | DC | C4'-C3'-O3' | 11.38 | 127.07 | 110.00 | 1 | 1 |
| F | 23 | DC | C4-C5-C6 | 11.24 | 100.74 | 117.60 | 1 | 1 |
| F | 21 | DC | O5'-C5'-C4' | 11.06 | 94.22 | 110.80 | 1 | 1 |
| B | 134 | ALA | C-N-CA | 11.04 | 141.57 | 121.70 | 1 | 1 |
| B | 156 | MET | N-CA-C | 11.02 | 141.86 | 111.00 | 1 | 1 |
| F | 7 | DC | C3'-O3'-P | 10.94 | 136.61 | 120.20 | 1 | 1 |
| D | 56 | THR | C-N-CA | 10.91 | 141.34 | 121.70 | 1 | 1 |
| F | 23 | DC | C1'-N1-C2 | 10.73 | 135.79 | 119.70 | 1 | 1 |
| F | 28 | DC | OP2-P-O5' | 10.65 | 76.06 | 108.00 | 1 | 1 |
| B | 155 | PHE | CA-C-N | 10.56 | 137.32 | 116.20 | 1 | 1 |
| F | 24 | DC | O4'-C1'-N1 | 10.55 | 124.23 | 108.40 | 1 | 1 |
| F | 21 | DC | C5'-C4'-C3' | 10.52 | 130.69 | 114.90 | 1 | 1 |
| F | 26 | DC | O3'-C3'-C2' | 10.48 | 95.78 | 111.50 | 1 | 1 |
| B | 130 | SER | C-N-CA | 10.46 | 140.54 | 121.70 | 1 | 1 |
| F | 27 | DC | C4'-C3'-C2' | 10.32 | 86.92 | 102.40 | 1 | 1 |
| D | 48 | TYR | C-N-CA | 10.30 | 140.24 | 121.70 | 1 | 1 |
| F | 29 | DC | C3'-O3'-P | 10.14 | 135.41 | 120.20 | 1 | 1 |
| F | 28 | DC | OP1-P-OP2 | 10.14 | 89.59 | 120.00 | 1 | 1 |
| B | 142 | PRO | N-CA-C | 9.99 | 137.08 | 112.10 | 1 | 1 |
| B | 138 | PRO | N-CA-C | 9.99 | 137.07 | 112.10 | 1 | 1 |
| F | 25 | DC | O5'-C5'-C4' | 9.95 | 125.73 | 110.80 | 1 | 1 |
| D | 121 | PHE | CA-CB-CG | 9.90 | 103.90 | 113.80 | 1 | 1 |
| B | 21 | PHE | CA-CB-CG | 9.83 | 103.97 | 113.80 | 1 | 1 |
| D | 62 | VAL | O-C-N | 9.80 | 107.32 | 123.00 | 1 | 1 |
| F | 23 | DC | C5'-C4'-O4' | 9.41 | 95.29 | 109.40 | 1 | 1 |
| B | 155 | PHE | N-CA-CB | 9.32 | 94.65 | 110.50 | 1 | 1 |
| F | 24 | DC | C2-N3-C4 | 9.25 | 106.12 | 120.00 | 1 | 1 |
| D | 63 | LYS | C-N-CA | 9.25 | 138.35 | 121.70 | 1 | 1 |
| F | 26 | DC | O3'-P-O5' | 9.19 | 90.21 | 104.00 | 1 | 1 |
| D | 62 | VAL | N-CA-C | 9.08 | 136.43 | 111.00 | 1 | 1 |
| B | 129 | ASN | CA-CB-CG | 8.93 | 121.53 | 112.60 | 1 | 1 |
| B | 218 | ASP | CA-CB-CG | 8.88 | 103.72 | 112.60 | 1 | 1 |
| B | 157 | PRO | O-C-N | 8.80 | 108.92 | 123.00 | 1 | 1 |
| F | 26 | DC | C4'-C3'-O3' | 8.68 | 96.97 | 110.00 | 1 | 1 |
| F | 23 | DC | N3-C4-C5 | 8.68 | 108.77 | 121.80 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| D | 55 | ALA | C-CA-CB | 8.59 | 97.62 | 110.50 | 1 | 1 |
| F | 27 | DC | O4'-C1'-C2' | 8.56 | 93.56 | 106.40 | 1 | 1 |
| F | 23 | DC | C2-N1-C6 | 8.56 | 107.76 | 120.60 | 1 | 1 |
| D | 101 | ASP | CA-CB-CG | 8.52 | 104.08 | 112.60 | 1 | 1 |
| F | 26 | DC | C2-N1-C6 | 8.48 | 107.88 | 120.60 | 1 | 1 |
| F | 26 | DC | P-O5'-C5' | 8.45 | 132.68 | 120.00 | 1 | 1 |
| F | 22 | DC | O4'-C1'-N1 | 8.43 | 95.76 | 108.40 | 1 | 1 |
| F | 22 | DC | O5'-C5'-C4' | 8.42 | 123.43 | 110.80 | 1 | 1 |
| F | 31 | DG | P-O5'-C5' | 8.37 | 107.44 | 120.00 | 1 | 1 |
| D | 62 | VAL | CA-C-N | 8.31 | 132.82 | 116.20 | 1 | 1 |

## 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 | 166.70 | 1843 |

*There are 1843 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are >= 0.4 Angstrom. The output is limited to 100 rows.*

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| D:181:TYR:CZ | E:13:DT:H5' | 1.71 | 1 | 1 |
| D:181:TYR:CE1 | E:13:DT:H5' | 1.62 | 1 | 1 |
| C:105:HIS:CE1 | D:53:ALA:CB | 1.62 | 1 | 1 |
| D:135:LYS:HD3 | E:16:DT:C4 | 1.59 | 1 | 1 |
| D:130:ARG:HB3 | E:15:DT:C3' | 1.56 | 1 | 1 |
| D:177:ASP:CB | F:33:DC:H5' | 1.54 | 1 | 1 |
| B:155:PHE:CA | B:155:PHE:N | 1.52 | 1 | 1 |
| D:177:ASP:HB2 | F:33:DC:C5' | 1.48 | 1 | 1 |
| C:105:HIS:CE1 | D:53:ALA:HB3 | 1.48 | 1 | 1 |
| D:130:ARG:HB3 | E:15:DT:C2' | 1.48 | 1 | 1 |
| B:157:PRO:C | B:158:ALA:N | 1.47 | 1 | 1 |
| D:181:TYR:CE1 | E:13:DT:C5' | 1.46 | 1 | 1 |
| B:156:MET:CA | B:156:MET:N | 1.44 | 1 | 1 |
| C:1:ASP:N | D:46:ARG:HH21 | 1.44 | 1 | 1 |
| B:156:MET:C | B:157:PRO:N | 1.41 | 1 | 1 |
| D:172:HIS:CE1 | E:10:DC:O2 | 1.40 | 1 | 1 |
| D:130:ARG:CG | E:16:DT:P | 1.40 | 1 | 1 |
| B:156:MET:C | B:156:MET:CA | 1.39 | 1 | 1 |
| D:130:ARG:HG2 | E:16:DT:P | 1.39 | 1 | 1 |
| D:137:LYS:CG | E:16:DT:H5' | 1.39 | 1 | 1 |
| B:157:PRO:CA | B:157:PRO:N | 1.38 | 1 | 1 |
| D:130:ARG:NH2 | E:16:DT:C6 | 1.38 | 1 | 1 |
| B:157:PRO:C | B:157:PRO:CA | 1.36 | 1 | 1 |
| D:130:ARG:CB | E:15:DT:H2" | 1.36 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| B:148:GLY:HA3 | D:46:ARG:CZ | 1.36 | 1 | 1 |
| B:148:GLY:HA3 | D:46:ARG:NH2 | 1.35 | 1 | 1 |
| D:175:TRP:CH2 | E:10:DC:H4' | 1.35 | 1 | 1 |
| D:130:ARG:HB2 | E:16:DT:OP1 | 1.34 | 1 | 1 |
| D:135:LYS:NZ | E:16:DT:O4 | 1.32 | 1 | 1 |
| D:130:ARG:CB | E:15:DT:C2' | 1.32 | 1 | 1 |
| D:135:LYS:CD | E:16:DT:C4 | 1.31 | 1 | 1 |
| B:148:GLY:C | D:46:ARG:HH12 | 1.30 | 1 | 1 |
| D:127:ASP:O | E:15:DT:C1' | 1.29 | 1 | 1 |
| D:126:CYS:HA | E:16:DT:OP2 | 1.28 | 1 | 1 |
| D:130:ARG:HG2 | E:16:DT:O5' | 1.28 | 1 | 1 |
| A:133:SER:OG | D:113:MET:SD | 1.27 | 1 | 1 |
| D:174:GLN:C | E:11:DT:H2" | 1.26 | 1 | 1 |
| B:155:PHE:C | B:155:PHE:CA | 1.26 | 1 | 1 |
| D:64:ALA:HB3 | E:15:DT:O5' | 1.26 | 1 | 1 |
| D:64:ALA:CB | E:15:DT:O5' | 1.25 | 1 | 1 |
| C:105:HIS:ND1 | D:54:ALA:N | 1.25 | 1 | 1 |
| A:85:LYS:HD2 | E:14:DT:C2 | 1.25 | 1 | 1 |
| D:137:LYS:NZ | E:16:DT:H2" | 1.24 | 1 | 1 |
| D:137:LYS:CG | E:16:DT:C5' | 1.24 | 1 | 1 |
| A:248:LEU:O | F:7:DC:H2' | 1.24 | 1 | 1 |
| D:168:LYS:CE | E:13:DT:O2 | 1.22 | 1 | 1 |
| D:175:TRP:CH2 | E:10:DC:C4' | 1.22 | 1 | 1 |
| D:175:TRP:N | E:11:DT:H2" | 1.22 | 1 | 1 |
| A:250:SER:OG | F:7:DC:OP1 | 1.22 | 1 | 1 |
| D:177:ASP:CB | F:33:DC:C5' | 1.21 | 1 | 1 |
| D:130:ARG:HB3 | E:15:DT:O3' | 1.21 | 1 | 1 |
| D:130:ARG:CG | E:16:DT:O5' | 1.20 | 1 | 1 |
| D:139:ILE:HD13 | E:14:DT:C5' | 1.20 | 1 | 1 |
| B:224:ASP:HB2 | D:39:ARG:NH2 | 1.20 | 1 | 1 |
| C:4:ASP:OD2 | D:48:TYR:CA | 1.20 | 1 | 1 |
| C:1:ASP:CA | D:46:ARG:HH21 | 1.20 | 1 | 1 |
| D:126:CYS:CA | E:16:DT:OP2 | 1.19 | 1 | 1 |
| D:130:ARG:CB | E:16:DT:OP1 | 1.19 | 1 | 1 |
| D:181:TYR:CZ | E:13:DT:C5' | 1.19 | 1 | 1 |
| D:130:ARG:CB | E:16:DT:P | 1.19 | 1 | 1 |
| D:173:SER:C | E:11:DT:H3' | 1.18 | 1 | 1 |
| C:1:ASP:N | D:46:ARG:NH2 | 1.18 | 1 | 1 |
| B:129:ASN:HB2 | F:28:DC:OP2 | 1.18 | 1 | 1 |
| D:67:LYS:HB2 | D:166:VAL:HB | 1.18 | 1 | 1 |
| B:148:GLY:CA | D:46:ARG:HH22 | 1.18 | 1 | 1 |
| D:141:LYS:HB3 | F:32:DC:OP2 | 1.18 | 1 | 1 |
| D:168:LYS:NZ | E:13:DT:O2 | 1.18 | 1 | 1 |
| D:106:GLU:CD | H:1:ZN2:ZN2 | 1.17 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| A:5:ILE:HD11 | A:49:GLY:HA3 | 1.17 | 1 | 1 |
| D:181:TYR:CG | E:14:DT:OP1 | 1.17 | 1 | 1 |
| D:130:ARG:CD | E:16:DT:O5' | 1.16 | 1 | 1 |
| D:179:LYS:HD2 | E:12:DT:C4' | 1.16 | 1 | 1 |
| A:11:TYR:OH | E:12:DT:C3' | 1.16 | 1 | 1 |
| D:172:HIS:CE1 | E:10:DC:C2 | 1.16 | 1 | 1 |
| D:108:CYS:SG | E:16:DT:H4' | 1.16 | 1 | 1 |
| D:149:LEU:HD13 | D:187:VAL:HG12 | 1.16 | 1 | 1 |
| D:137:LYS:HG2 | E:16:DT:C5' | 1.15 | 1 | 1 |
| D:125:THR:O | E:16:DT:OP2 | 1.15 | 1 | 1 |
| A:38:LYS:HD3 | A:58:GLU:HB2 | 1.14 | 1 | 1 |
| D:135:LYS:HD3 | E:16:DT:C5 | 1.14 | 1 | 1 |
| D:172:HIS:NE2 | E:10:DC:C2 | 1.14 | 1 | 1 |
| D:134:ASP:H | E:15:DT:H73 | 1.13 | 1 | 1 |
| D:169:ASN:O | E:13:DT:OP1 | 1.13 | 1 | 1 |
| A:201:VAL:HG13 | A:211:VAL:HG13 | 1.13 | 1 | 1 |
| B:191:LYS:HE2 | B:194:SER:HB3 | 1.13 | 1 | 1 |
| A:91:LYS:HE2 | A:93:ASP:HB3 | 1.13 | 1 | 1 |
| D:168:LYS:HE3 | E:13:DT:O2 | 1.13 | 1 | 1 |
| D:181:TYR:CZ | E:13:DT:H3' | 1.13 | 1 | 1 |
| A:131:LYS:HD2 | A:134:LEU:HB2 | 1.12 | 1 | 1 |
| B:155:PHE:CB | B:226:GLU:HB3 | 1.12 | 1 | 1 |
| D:126:CYS:HA | E:16:DT:P | 1.12 | 1 | 1 |
| A:138:ILE:HD12 | A:200:ARG:HD2 | 1.12 | 1 | 1 |
| A:86:GLN:OE1 | D:117:LEU:CG | 1.12 | 1 | 1 |
| A:248:LEU:O | F:7:DC:C2' | 1.12 | 1 | 1 |
| C:32:ILE:HG13 | C:41:LEU:HD23 | 1.12 | 1 | 1 |
| D:131:ASP:O | E:15:DT:C7 | 1.11 | 1 | 1 |
| D:177:ASP:HB3 | F:33:DC:H5' | 1.11 | 1 | 1 |
| D:181:TYR:HH | E:13:DT:C5' | 1.11 | 1 | 1 |
| D:127:ASP:H | E:15:DT:H2' | 1.11 | 1 | 1 |
| B:148:GLY:CA | D:46:ARG:NH2 | 1.11 | 1 | 1 |

## 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 | 1003 | 897 | 53 | 53 |

*There are 53 unique backbone outliers. Detailed list of outliers are tabulated below.*

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 10 | PRO | 1 |
| A | 38 | LYS | 1 |
| A | 64 | PHE | 1 |

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 79 | THR | 1 |
| A | 116 | VAL | 1 |
| A | 192 | PRO | 1 |
| A | 199 | ALA | 1 |
| A | 208 | SER | 1 |
| A | 221 | PRO | 1 |
| A | 223 | ILE | 1 |
| A | 257 | ASN | 1 |
| A | 280 | PHE | 1 |
| B | 67 | THR | 1 |
| B | 96 | LYS | 1 |
| B | 129 | ASN | 1 |
| B | 133 | SER | 1 |
| B | 153 | ASN | 1 |
| B | 154 | SER | 1 |
| B | 155 | PHE | 1 |
| B | 157 | PRO | 1 |
| B | 158 | ALA | 1 |
| B | 195 | VAL | 1 |
| B | 196 | SER | 1 |
| B | 215 | VAL | 1 |
| C | 21 | LYS | 1 |
| C | 37 | LYS | 1 |
| C | 64 | ILE | 1 |
| C | 90 | HIS | 1 |
| C | 108 | PRO | 1 |
| C | 112 | PRO | 1 |
| D | 18 | ALA | 1 |
| D | 19 | GLU | 1 |
| D | 31 | LYS | 1 |
| D | 45 | ALA | 1 |
| D | 46 | ARG | 1 |
| D | 49 | SER | 1 |
| D | 51 | THR | 1 |
| D | 52 | ALA | 1 |
| D | 53 | ALA | 1 |
| D | 54 | ALA | 1 |
| D | 55 | ALA | 1 |
| D | 60 | ALA | 1 |
| D | 61 | ASN | 1 |
| D | 90 | VAL | 1 |
| D | 91 | VAL | 1 |
| D | 92 | HIS | 1 |

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| D | 97 | VAL | 1 |
| D | 98 | MET | 1 |
| D | 100 | PHE | 1 |
| D | 123 | LEU | 1 |
| D | 160 | PRO | 1 |
| D | 197 | GLN | 1 |
| D | 234 | VAL | 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 | 882 | 709 | 91 | 82 |

*There are 82 unique sidechain outliers. Detailed list of outliers are tabulated below.*

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 1 | LYS | 1 |
| A | 5 | ILE | 1 |
| A | 65 | PRO | 1 |
| A | 70 | ASN | 1 |
| A | 81 | LYS | 1 |
| A | 91 | LYS | 1 |
| A | 99 | ASN | 1 |
| A | 131 | LYS | 1 |
| A | 138 | ILE | 1 |
| A | 155 | ASN | 1 |
| A | 161 | LYS | 1 |
| A | 162 | ARG | 1 |
| A | 166 | LEU | 1 |
| A | 211 | VAL | 1 |
| A | 223 | ILE | 1 |
| A | 228 | LYS | 1 |
| A | 286 | VAL | 1 |
| A | 291 | LYS | 1 |
| A | 295 | MET | 1 |
| A | 302 | GLN | 1 |
| A | 351 | GLN | 1 |
| A | 357 | ILE | 1 |
| A | 384 | ASN | 1 |
| A | 395 | LYS | 1 |
| A | 413 | LYS | 1 |
| A | 418 | ARG | 1 |
| A | 422 | ARG | 1 |
| A | 428 | ILE | 1 |
| B | 23 | ILE | 1 |

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| B | 28 | ILE | 1 |
| B | 38 | ARG | 1 |
| B | 59 | MET | 1 |
| B | 84 | LYS | 1 |
| B | 99 | VAL | 1 |
| B | 102 | LYS | 1 |
| B | 116 | ILE | 1 |
| B | 128 | LYS | 1 |
| B | 171 | LEU | 1 |
| B | 173 | LYS | 1 |
| B | 187 | LYS | 1 |
| B | 191 | LYS | 1 |
| B | 211 | ILE | 1 |
| C | 7 | ARG | 1 |
| C | 19 | ILE | 1 |
| C | 41 | LEU | 1 |
| C | 47 | LYS | 1 |
| C | 77 | ILE | 1 |
| C | 96 | LEU | 1 |
| C | 103 | ILE | 1 |
| D | 1 | MET | 1 |
| D | 19 | GLU | 1 |
| D | 25 | ARG | 1 |
| D | 40 | GLN | 1 |
| D | 51 | THR | 1 |
| D | 61 | ASN | 1 |
| D | 68 | ILE | 1 |
| D | 69 | ILE | 1 |
| D | 83 | GLU | 1 |
| D | 89 | LYS | 1 |
| D | 93 | GLN | 1 |
| D | 98 | MET | 1 |
| D | 117 | LEU | 1 |
| D | 119 | ASN | 1 |
| D | 135 | LYS | 1 |
| D | 137 | LYS | 1 |
| D | 151 | LYS | 1 |
| D | 157 | LYS | 1 |
| D | 159 | GLU | 1 |
| D | 163 | LYS | 1 |
| D | 167 | LYS | 1 |
| D | 178 | MET | 1 |
| D | 179 | LYS | 1 |
| D | 197 | GLN | 1 |

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| D | 198 | GLU | 1 |
| D | 204 | LYS | 1 |
| D | 212 | GLU | 1 |
| D | 215 | LYS | 1 |
| D | 218 | LYS | 1 |
| D | 222 | LYS | 1 |
| D | 224 | LYS | 1 |
| D | 235 | TRP | 1 |
| D | 236 | LYS | 1 |

## 5. Fit to Data Used for Modeling Assessment ?

SAS data used in this integrative model could not be validated as the sasCIF file is currently unavailable or incomplete.

## 6. Fit to Data Used for Validation Assessment ?

Validation for this section is under development.

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