# Full wwPDB NMR Structure Validation Report (i)

Feb 14, 2022 – 10:44 AM EST

| | | |
|---|---|---|
| PDB ID | : | 1K2N |
| Title | : | Solution Structure of the FHA2 domain of Rad53 Complexed with a Phosphothreonyl Peptide Derived from Rad9 |
| Authors | : | Byeon, I.-J.L.; Yongkiettrakul, S.; Tsai, M.-D. |
| Deposited on | : | 2001-09-28 |

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

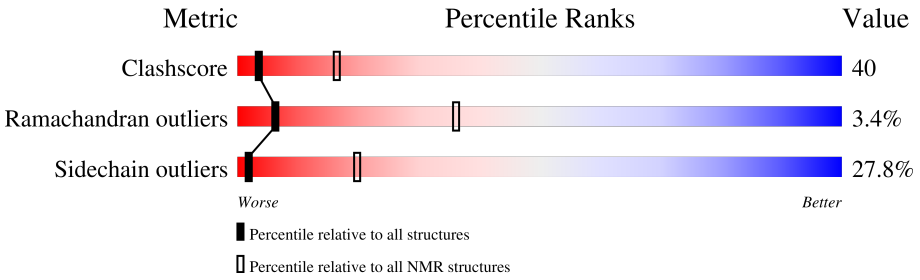
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.26 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.26 |

# 1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 158 | 23% 47% 8% • 21% |
| 2 | P | 9 | 100% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:576-A:630, A:644-A:699, A:716-A:729 (125) | 0.20 | 13 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2701 atoms, of which 1349 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein Kinase SPK1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 158 | 2551 | 806 | 1277 | 222 | 239 | 7 | 0 |

- Molecule 2 is a protein called DNA repair protein Rad9.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | |
| 2 | P | 9 | 150 | 46 | 72 | 10 | 21 | 1 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| P | 603 | TPO | THR | modified residue | UNP P14737 |

# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Protein Kinase SPK1

Chain A: 23% 47% 8% • 21%

• Molecule 2: DNA repair protein Rad9

Chain P: 100%

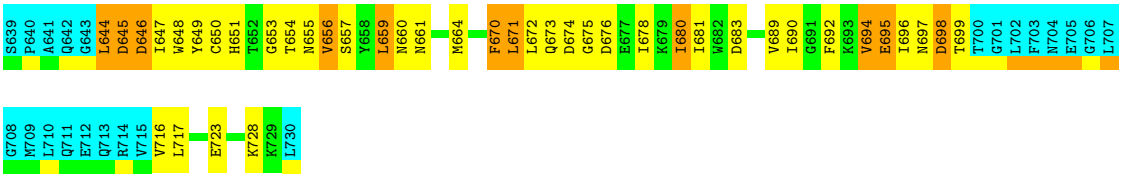
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

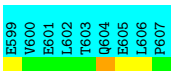
• Molecule 1: Protein Kinase SPK1

Chain A: 28% 39% 12% 21%




• Molecule 2: DNA repair protein Rad9

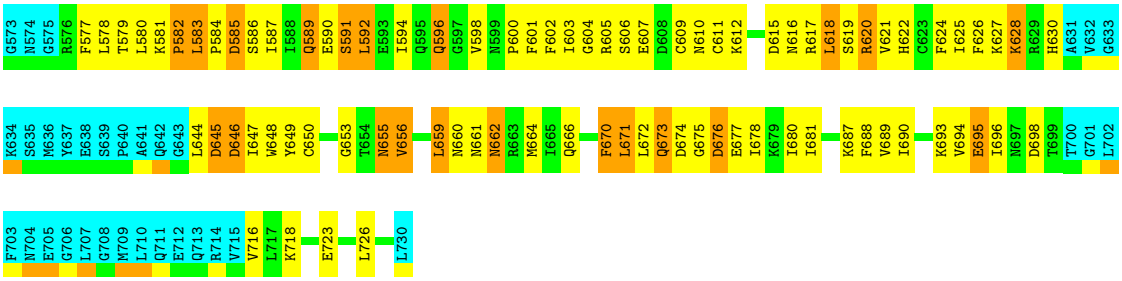
Chain P: 100%




### 4.2.2 Score per residue for model 2

• Molecule 1: Protein Kinase SPK1

Chain A: 26% 40% 13% 21%



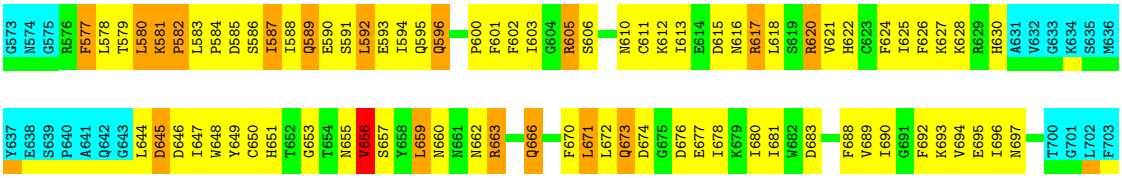

• Molecule 2: DNA repair protein Rad9

Chain P: 100%

### 4.2.3 Score per residue for model 3

• Molecule 1: Protein Kinase SPK1

Chain A: 24% 44% 11% • 21%



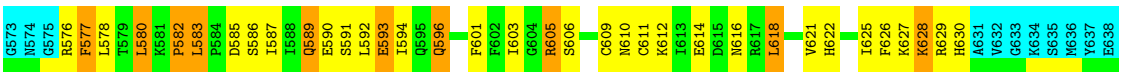
• Molecule 2: DNA repair protein Rad9

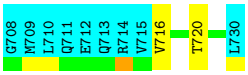
Chain P: 100%

### 4.2.4 Score per residue for model 4

• Molecule 1: Protein Kinase SPK1

Chain A: 32% 35% 13% 21%





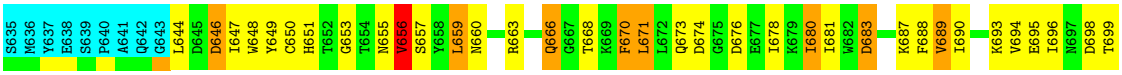

• Molecule 2: DNA repair protein Rad9

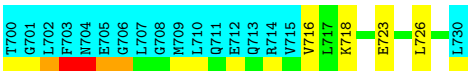
Chain P: 100%

### 4.2.5 Score per residue for model 5

• Molecule 1: Protein Kinase SPK1

Chain A: 25% 41% 12% • 21%




• Molecule 2: DNA repair protein Rad9

Chain P: 100%

E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.6 Score per residue for model 6

- Molecule 1: Protein Kinase SPK1

Chain A: 23% 41% 13% • 21%

G573 N574 G575 R576 F577 L578 T579 L580 K581 P582 L583 P584 D585 S586 I587 I588 Q589 E590 S591 L592 E593 I594 Q595 Q596 G597 P600 F601 F602 I603 G604 R605 S606 E607 D608 C609 N610 C611 K612 I613 E614 D615 N616 R617 L618 H622 C623 F624 I625 F626 K627 K628 R629 H630 A631 V632 G633 K634 S635

M636 Y637 E638 S639 P640 A641 Q642 G643 L644 D645 D646 I647 W648 Y649 C650 H651 T652 G653 T654 N655 V656 S657 Y658 L659 N660 N661 N662 R663 M664 F670 L671 L672 Q673 D674 G675 D676 E677 I678 K679 I680 I681 W682 D683 K684 F688 V689 I690 G691 F692 K693 V694 E695 I696 N697 D698 T699 T700 G701

L702 F703 N704 E705 G706 L707 G708 M709 L710 Q711 E712 Q713 R714 V715 V716 L717 K718 E723 K724 D725 L726 V727 L730

- Molecule 2: DNA repair protein Rad9

Chain P: 100%

E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.7 Score per residue for model 7

- Molecule 1: Protein Kinase SPK1

Chain A: 25% 42% 11% • 21%

G573 N574 G575 R576 F577 L578 T579 L580 K581 P582 L583 P584 D585 S586 I587 I588 Q589 E590 S591 L592 E593 I594 Q595 Q596 G597 V598 N599 P600 F601 F602 I603 G604 R605 S606 C611 K612 I613 E614 D615 N616 R617 L618 S619 R620 V621 H622 C623 F624 I625 F626 K627 K628 R629 H630 A631 V632 G633 K634 S635

M636 Y637 E638 S639 P640 A641 Q642 G643 L644 D645 D646 I647 W648 Y649 C650 H651 T652 G653 T654 N655 V656 S657 Y658 L659 N660 R663 Q666 F670 L671 L672 Q673 D674 G675 D676 E677 I678 K679 I680 I681 K684 N685 N686 K687 F688 V689 I690 G691 F692 K693 V694 E695 I696 N697 D698 T699 T700

G701 L702 F703 N704 E705 G706 L707 G708 M709 L710 Q711 E712 Q713 R714 V715 V716 L717 K718 E723 L726 L730

- Molecule 2: DNA repair protein Rad9

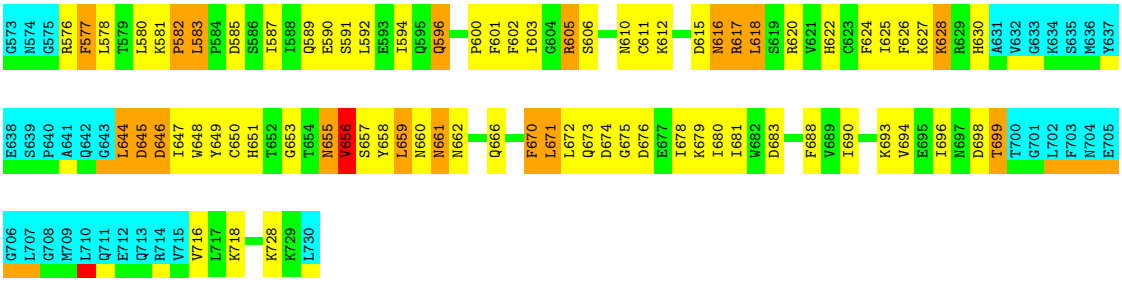
Chain P: 100%

E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.8 Score per residue for model 8

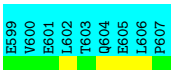
- Molecule 1: Protein Kinase SPK1

Chain A: 31% 36% 11% • 21%




- Molecule 2: DNA repair protein Rad9

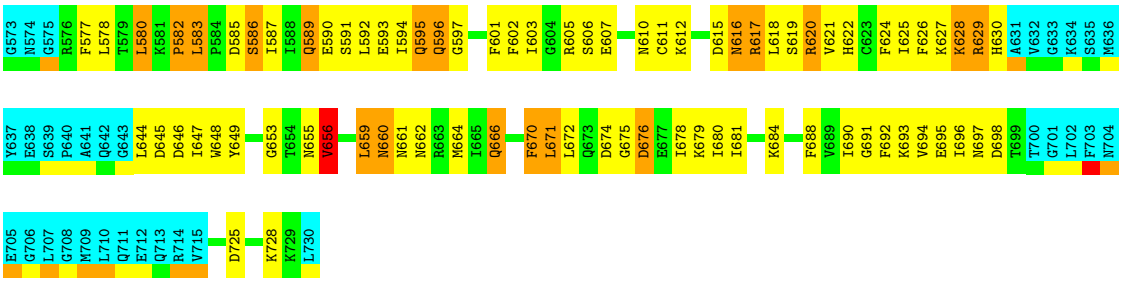
Chain P: 100%




### 4.2.9 Score per residue for model 9

- Molecule 1: Protein Kinase SPK1

Chain A: 29% 38% 11% • 21%




- Molecule 2: DNA repair protein Rad9

Chain P: 100%

### 4.2.10 Score per residue for model 10

- Molecule 1: Protein Kinase SPK1

Chain A: 21% 44% 14% • 21%

G573 N574 G575 R576 F577 L578 T579 L580 K581 P582 L583 P584 D585 S586 I587 I588 Q589 E590 S591 L592 E593 I594 Q595 Q596 G597 V598 N599 P600 F601 F602 I603 G604 R605 S606 E607 N610 C611 K612 I613 E614 D615 N616 R617 L618 S619 R620 V621 H622 C623 F624 I625 F626 K627 K628 R629 H630 A631 V632 G633

K634 S635 M636 Y637 E638 S639 P640 A641 Q642 G643 L644 D645 D646 I647 W648 Y649 C650 H651 T652 G653 T654 N655 V656 S657 Y658 L659 N660 N661 N662 Q666 K669 F670 L671 L672 Q673 D674 G675 D676 E677 I678 K679 I680 I681 N685 N686 K687 F688 V689 I690 K693 V694 E695 I696 N697 D698 T699

T700 G701 L702 F703 N704 E705 G706 L707 G708 M709 L710 Q711 E712 Q713 R714 V715 V716 L717 K718 E722 V727 L730

• Molecule 2: DNA repair protein Rad9

Chain P: 100%

E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.11 Score per residue for model 11

• Molecule 1: Protein Kinase SPK1

Chain A: 22% 44% 13% • 21%

G573 N574 G575 R576 F577 L578 T579 L580 K581 P582 L583 P584 D585 S586 I587 I588 Q589 E590 S591 L592 E593 I594 Q595 Q596 P600 F601 F602 I603 G604 R605 S606 N610 C611 K612 I613 E614 D615 N616 R617 L618 S619 R620 V621 H622 C623 F624 I625 F626 K627 K628 R629 H630 A631 V632 G633 K634 S635 M636

Y637 E638 S639 P640 A641 Q642 G643 L644 D645 D646 I647 W648 Y649 C650 H651 T652 G653 T654 N655 V656 S657 Y658 L659 N660 N661 Q666 G667 T668 K669 F670 L671 L672 Q673 D674 G675 D676 E677 I678 K679 I680 I681 W682 D683 N686 K687 F688 V689 I690 G691 F692 K693 V694 E695 I696 N697 D698 T699 T700

G701 L702 F703 N704 E705 G706 L707 G708 M709 L710 Q711 E712 Q713 R714 V715 V716 L717 K718 Q719 T720 E723 L730

• Molecule 2: DNA repair protein Rad9

Chain P: 100%

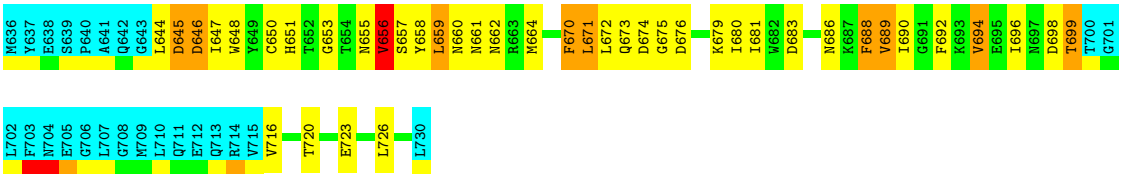
E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.12 Score per residue for model 12

• Molecule 1: Protein Kinase SPK1

Chain A: 30% 37% 11% • 21%

G573 N574 G575 R576 F577 L578 T579 L580 K581 P582 L583 P584 I587 I588 Q589 E590 S591 L592 E593 I594 Q595 Q596 G597 V598 N599 P600 F601 F602 I603 G604 R605 S606 E607 D608 G609 N610 C611 K612 I613 E614 D615 N616 R617 L618 H622 C623 F624 I625 F626 K627 K628 R629 H630 A631 V632 G633 K634 S635



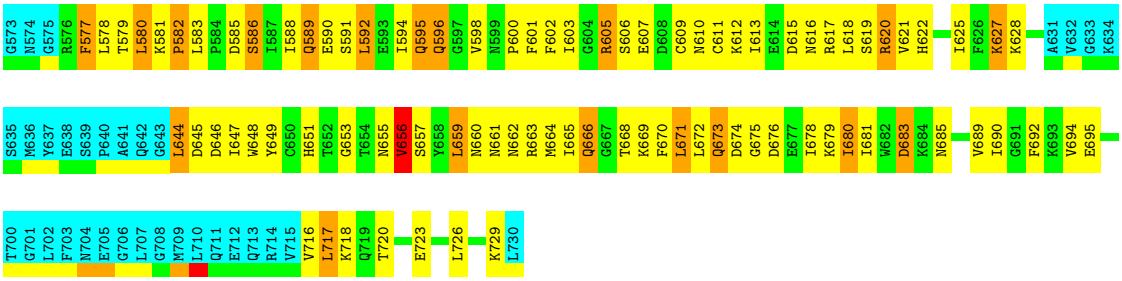

• Molecule 2: DNA repair protein Rad9

Chain P: 100%

### 4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Protein Kinase SPK1

Chain A: 24% 42% 12% • 21%



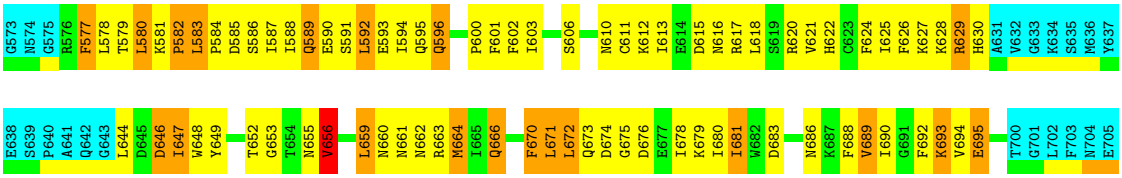

• Molecule 2: DNA repair protein Rad9

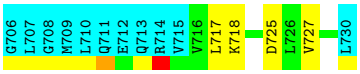
Chain P: 100%

### 4.2.14 Score per residue for model 14

• Molecule 1: Protein Kinase SPK1

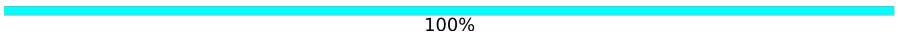
Chain A: 27% 39% 13% • 21%






• Molecule 2: DNA repair protein Rad9

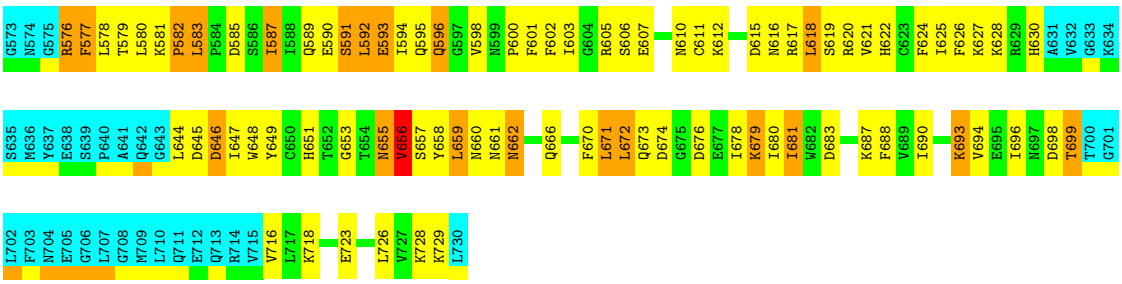
Chain P:



### 4.2.15 Score per residue for model 15

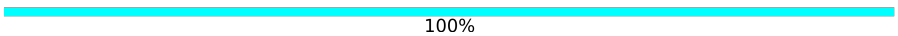
• Molecule 1: Protein Kinase SPK1

Chain A:




• Molecule 2: DNA repair protein Rad9

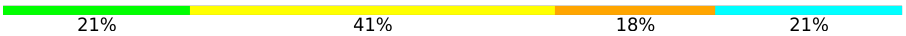
Chain P:

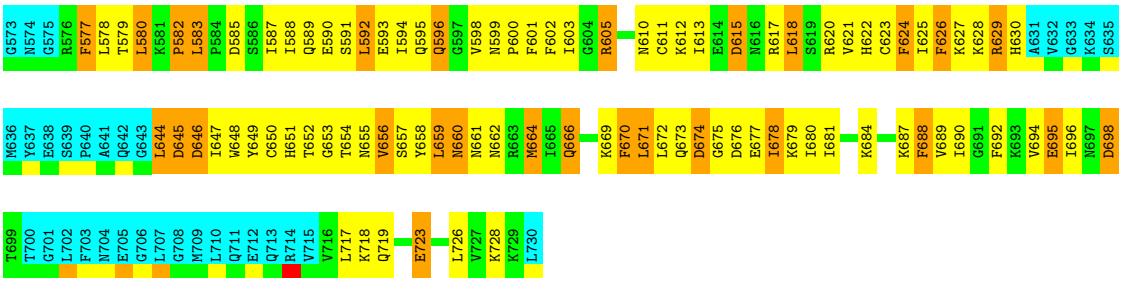


### 4.2.16 Score per residue for model 16

• Molecule 1: Protein Kinase SPK1

Chain A:




• Molecule 2: DNA repair protein Rad9

Chain P: 100%

E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.17 Score per residue for model 17

- Molecule 1: Protein Kinase SPK1

Chain A: 28% 34% 16% • 21%

G573 N574 G575 R576 F577 L578 T579 L580 K581 P582 L583 P584 D585 S586 I587 I588 Q589 E590 S591 L592 E593 I594 Q595 Q596 P600 F601 F602 I603 G604 R605 S606 E607 N610 C611 K612 I613 E614 D615 N616 R617 L618 S619 R620 V621 H622 C623 F624 I625 F626 K627 K628 R629 H630 A631 V632 G633 K634 S635

M636 Y637 E638 S639 P640 A641 Q642 G643 L644 D645 D646 I647 W648 Y649 C650 H651 T652 G653 T654 N655 V656 S657 Y658 L659 N660 N661 N662 Q666 G667 T668 K669 F670 L671 L672 Q673 D676 E677 I678 K679 I680 I681 W682 D683 K687 F688 F692 K693 V694 E695 I696 N697 D698 T699 T700 G701 L702

F703 N704 E705 G706 L707 G708 M709 L710 Q711 E712 Q713 R714 V715 V716 L717 K718 E723 L726 L730

- Molecule 2: DNA repair protein Rad9

Chain P: 100%

E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.18 Score per residue for model 18

- Molecule 1: Protein Kinase SPK1

Chain A: 25% 41% 13% 21%

G573 N574 G575 R576 F577 L578 T579 L580 K581 P582 L583 I587 E590 S591 L592 E593 I594 Q595 Q596 G597 V598 N599 P600 F601 F602 I603 G604 R605 S606 E607 D608 C609 N610 C611 K612 I613 E614 D615 N616 R617 L618 S619 R620 V621 H622 C623 F624 I625 F626 K627 K628 R629 H630 A631 V632 G633 K634 S635

M636 Y637 E638 S639 P640 A641 Q642 G643 L644 D645 D646 I647 W648 Y649 T652 G653 T654 N655 V656 S657 Y658 L659 N660 N661 N662 R663 Q666 F670 L671 L672 Q673 D674 G675 D676 E677 I678 K679 I680 I681 W682 D683 K684 K687 I690 G691 F692 K693 V694 E695 I696 T699 T700 G701 L702

F703 N704 E705 G706 L707 G708 M709 L710 Q711 E712 Q713 R714 V715 V716 L717 K718 Q719 T720 E723 K724 D725 L726 L730

- Molecule 2: DNA repair protein Rad9

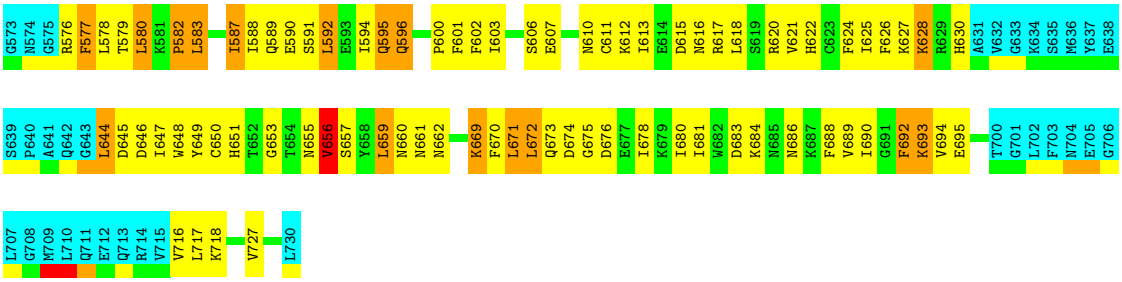
Chain P: 100%

E599 V600 E601 L602 T603 Q604 E605 L606 P607

### 4.2.19 Score per residue for model 19

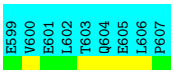
- Molecule 1: Protein Kinase SPK1

Chain A: 28% 40% 10% • 21%




- Molecule 2: DNA repair protein Rad9

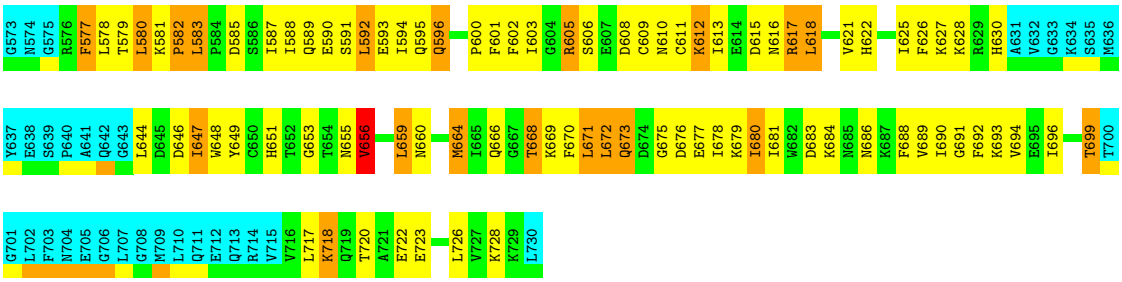
Chain P: 100%




### 4.2.20 Score per residue for model 20

- Molecule 1: Protein Kinase SPK1

Chain A: 25% 41% 13% • 21%




- Molecule 2: DNA repair protein Rad9

Chain P: 100%

# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *The complex structures are generated using a total of 3369 restraints, 3181 distance restraints, and 188 TALOS-derived dihedral angle restraints..*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

| Software name | Classification | Version |
|---|---|---|
| X-PLOR | structure solution | 3.851 |
| X-PLOR | refinement | 3.851 |

No chemical shift data was provided.

# 6 Model quality (i)

## 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 1034 | 1044 | 1041 | 83±8 |
| 2 | P | 0 | 0 | 0 | 0±0 |
| All | All | 20680 | 20880 | 20820 | 1652 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:578:LEU:HD11 | 1:A:694:VAL:HG13 | 1.04 | 1.26 | 12 | 10 |
| 1:A:578:LEU:HD21 | 1:A:694:VAL:HG13 | 1.03 | 1.29 | 16 | 2 |
| 1:A:580:LEU:HD22 | 1:A:694:VAL:HG22 | 0.95 | 1.34 | 7 | 2 |
| 1:A:578:LEU:HD12 | 1:A:647:ILE:HD13 | 0.95 | 1.35 | 14 | 10 |
| 1:A:594:ILE:HD11 | 1:A:625:ILE:HD12 | 0.93 | 1.41 | 6 | 10 |
| 1:A:577:PHE:CZ | 1:A:647:ILE:HG21 | 0.87 | 2.05 | 19 | 9 |
| 1:A:592:LEU:HD21 | 1:A:613:ILE:HD11 | 0.86 | 1.46 | 7 | 10 |
| 1:A:578:LEU:CD1 | 1:A:694:VAL:HG13 | 0.86 | 1.99 | 17 | 9 |
| 1:A:648:TRP:CH2 | 1:A:671:LEU:HD22 | 0.86 | 2.05 | 2 | 15 |
| 1:A:659:LEU:HD13 | 1:A:678:ILE:HG22 | 0.84 | 1.49 | 15 | 4 |
| 1:A:580:LEU:CD2 | 1:A:694:VAL:HG23 | 0.84 | 2.03 | 1 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:672:LEU:HD13 | 1:A:694:VAL:HG21 | 0.84 | 1.47 | 10 | 13 |
| 1:A:681:ILE:HG22 | 1:A:690:ILE:HG22 | 0.83 | 1.48 | 19 | 1 |
| 1:A:578:LEU:HD23 | 1:A:594:ILE:HD12 | 0.83 | 1.51 | 7 | 3 |
| 1:A:659:LEU:HD22 | 1:A:678:ILE:HG22 | 0.81 | 1.52 | 11 | 1 |
| 1:A:648:TRP:CZ3 | 1:A:671:LEU:HD22 | 0.80 | 2.12 | 19 | 14 |
| 1:A:662:ASN:OD1 | 1:A:716:VAL:HG23 | 0.77 | 1.78 | 15 | 3 |
| 1:A:621:VAL:HG11 | 1:A:727:VAL:HG23 | 0.77 | 1.55 | 14 | 3 |
| 1:A:580:LEU:HD11 | 1:A:594:ILE:HD11 | 0.77 | 1.55 | 10 | 1 |
| 1:A:681:ILE:HG22 | 1:A:690:ILE:HB | 0.77 | 1.56 | 12 | 12 |
| 1:A:598:VAL:HG11 | 1:A:610:ASN:OD1 | 0.76 | 1.80 | 12 | 6 |
| 1:A:578:LEU:HD13 | 1:A:647:ILE:HD13 | 0.76 | 1.55 | 9 | 6 |
| 1:A:580:LEU:HD12 | 1:A:594:ILE:HD11 | 0.76 | 1.57 | 15 | 5 |
| 1:A:580:LEU:CD2 | 1:A:694:VAL:HG22 | 0.76 | 2.09 | 10 | 2 |
| 1:A:580:LEU:HD21 | 1:A:694:VAL:HG23 | 0.76 | 1.58 | 12 | 4 |
| 1:A:622:HIS:CD2 | 1:A:680:ILE:HG23 | 0.76 | 2.15 | 18 | 13 |
| 1:A:578:LEU:HD22 | 1:A:594:ILE:HD12 | 0.75 | 1.55 | 18 | 7 |
| 1:A:580:LEU:HD22 | 1:A:694:VAL:CG2 | 0.74 | 2.12 | 7 | 2 |
| 1:A:578:LEU:HD12 | 1:A:647:ILE:CD1 | 0.73 | 2.12 | 18 | 9 |
| 1:A:620:ARG:HG2 | 1:A:621:VAL:HG23 | 0.73 | 1.59 | 5 | 5 |
| 1:A:578:LEU:HD23 | 1:A:579:THR:N | 0.73 | 1.98 | 14 | 8 |
| 1:A:592:LEU:HD13 | 1:A:611:CYS:SG | 0.72 | 2.25 | 7 | 13 |
| 1:A:579:THR:HG23 | 1:A:593:GLU:HG3 | 0.72 | 1.58 | 7 | 1 |
| 1:A:659:LEU:HD22 | 1:A:678:ILE:CG2 | 0.72 | 2.13 | 11 | 1 |
| 1:A:587:ILE:HD13 | 1:A:688:PHE:CE1 | 0.72 | 2.20 | 15 | 5 |
| 1:A:603:ILE:HG23 | 1:A:611:CYS:SG | 0.72 | 2.25 | 9 | 20 |
| 1:A:578:LEU:HD11 | 1:A:694:VAL:CG1 | 0.71 | 2.14 | 8 | 13 |
| 1:A:647:ILE:HD12 | 1:A:672:LEU:CB | 0.71 | 2.15 | 11 | 10 |
| 1:A:577:PHE:CE1 | 1:A:647:ILE:HG21 | 0.71 | 2.20 | 16 | 10 |
| 1:A:587:ILE:HD11 | 1:A:690:ILE:HD11 | 0.70 | 1.62 | 7 | 5 |
| 1:A:580:LEU:CD1 | 1:A:594:ILE:HD11 | 0.70 | 2.16 | 15 | 8 |
| 1:A:680:ILE:HD12 | 1:A:692:PHE:CE2 | 0.70 | 2.22 | 3 | 5 |
| 1:A:646:ASP:OD2 | 1:A:671:LEU:HD11 | 0.70 | 1.86 | 9 | 3 |
| 1:A:578:LEU:HD22 | 1:A:647:ILE:CD1 | 0.70 | 2.16 | 17 | 7 |
| 1:A:681:ILE:HG22 | 1:A:690:ILE:CG2 | 0.70 | 2.16 | 19 | 1 |
| 1:A:578:LEU:HD22 | 1:A:647:ILE:HD13 | 0.69 | 1.64 | 7 | 8 |
| 1:A:579:THR:HG23 | 1:A:593:GLU:CG | 0.69 | 2.18 | 7 | 1 |
| 1:A:594:ILE:HD11 | 1:A:625:ILE:CD1 | 0.69 | 2.15 | 6 | 8 |
| 1:A:578:LEU:HD21 | 1:A:694:VAL:CG1 | 0.68 | 2.16 | 16 | 1 |
| 1:A:577:PHE:CB | 1:A:596:GLN:HA | 0.67 | 2.19 | 7 | 1 |
| 1:A:659:LEU:HD21 | 1:A:672:LEU:CD2 | 0.67 | 2.20 | 19 | 16 |
| 1:A:586:SER:O | 1:A:589:GLN:NE2 | 0.67 | 2.28 | 2 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:592:LEU:HD22 | 1:A:611:CYS:SG | 0.67 | 2.28 | 19 | 13 |
| 1:A:623:CYS:SG | 1:A:680:ILE:HD11 | 0.67 | 2.29 | 17 | 1 |
| 1:A:618:LEU:HD23 | 1:A:618:LEU:O | 0.67 | 1.90 | 2 | 3 |
| 1:A:588:ILE:HD13 | 1:A:613:ILE:HG23 | 0.67 | 1.67 | 7 | 5 |
| 1:A:672:LEU:CD1 | 1:A:694:VAL:HG21 | 0.66 | 2.19 | 10 | 3 |
| 1:A:664:MET:CE | 1:A:716:VAL:HG13 | 0.66 | 2.20 | 6 | 1 |
| 1:A:578:LEU:HD21 | 1:A:694:VAL:HG22 | 0.66 | 1.65 | 4 | 9 |
| 1:A:587:ILE:CD1 | 1:A:690:ILE:HD11 | 0.65 | 2.22 | 7 | 2 |
| 1:A:594:ILE:CD1 | 1:A:625:ILE:HD12 | 0.65 | 2.22 | 2 | 6 |
| 1:A:674:ASP:HB2 | 1:A:696:ILE:HD12 | 0.65 | 1.68 | 6 | 7 |
| 1:A:580:LEU:HG | 1:A:694:VAL:HG22 | 0.65 | 1.66 | 5 | 10 |
| 1:A:580:LEU:HD23 | 1:A:678:ILE:HD11 | 0.65 | 1.68 | 16 | 1 |
| 1:A:615:ASP:CB | 1:A:618:LEU:HD22 | 0.65 | 2.21 | 10 | 2 |
| 1:A:583:LEU:HD12 | 1:A:693:LYS:HB2 | 0.64 | 1.67 | 18 | 3 |
| 1:A:578:LEU:HD13 | 1:A:647:ILE:CD1 | 0.64 | 2.23 | 9 | 6 |
| 1:A:603:ILE:CD1 | 1:A:625:ILE:HD12 | 0.64 | 2.22 | 14 | 7 |
| 1:A:594:ILE:HG23 | 1:A:601:PHE:CD1 | 0.64 | 2.28 | 7 | 14 |
| 1:A:587:ILE:HG22 | 1:A:690:ILE:HG12 | 0.63 | 1.70 | 2 | 1 |
| 1:A:622:HIS:O | 1:A:653:GLY:N | 0.63 | 2.32 | 4 | 20 |
| 1:A:644:LEU:N | 1:A:644:LEU:HD23 | 0.63 | 2.09 | 1 | 6 |
| 1:A:649:TYR:CE1 | 1:A:678:ILE:HD12 | 0.63 | 2.29 | 15 | 2 |
| 1:A:659:LEU:HG | 1:A:678:ILE:HG22 | 0.63 | 1.71 | 4 | 1 |
| 1:A:580:LEU:HD11 | 1:A:625:ILE:HD11 | 0.63 | 1.68 | 8 | 4 |
| 1:A:647:ILE:HD12 | 1:A:672:LEU:HB2 | 0.62 | 1.70 | 1 | 13 |
| 1:A:615:ASP:HB3 | 1:A:618:LEU:HD22 | 0.62 | 1.71 | 10 | 2 |
| 1:A:615:ASP:CB | 1:A:618:LEU:HD13 | 0.62 | 2.24 | 19 | 2 |
| 1:A:680:ILE:HD12 | 1:A:692:PHE:CZ | 0.62 | 2.30 | 19 | 3 |
| 1:A:682:TRP:CD1 | 1:A:689:VAL:CG1 | 0.62 | 2.82 | 4 | 1 |
| 1:A:583:LEU:HD12 | 1:A:585:ASP:HB2 | 0.62 | 1.69 | 8 | 10 |
| 1:A:664:MET:HE1 | 1:A:716:VAL:HG13 | 0.61 | 1.72 | 6 | 1 |
| 1:A:609:CYS:SG | 1:A:621:VAL:HG22 | 0.61 | 2.35 | 5 | 6 |
| 1:A:577:PHE:CE2 | 1:A:647:ILE:HG21 | 0.61 | 2.30 | 13 | 8 |
| 1:A:580:LEU:HD11 | 1:A:625:ILE:CD1 | 0.61 | 2.25 | 8 | 5 |
| 1:A:649:TYR:CD2 | 1:A:678:ILE:HD13 | 0.61 | 2.30 | 5 | 6 |
| 1:A:602:PHE:CE2 | 1:A:624:PHE:CZ | 0.61 | 2.88 | 16 | 2 |
| 1:A:624:PHE:O | 1:A:650:CYS:N | 0.60 | 2.32 | 17 | 12 |
| 1:A:603:ILE:HD12 | 1:A:624:PHE:HA | 0.60 | 1.74 | 6 | 10 |
| 1:A:582:PRO:HD2 | 1:A:590:GLU:O | 0.60 | 1.97 | 11 | 20 |
| 1:A:621:VAL:HG11 | 1:A:727:VAL:CG2 | 0.59 | 2.28 | 14 | 1 |
| 1:A:580:LEU:HD21 | 1:A:625:ILE:HD11 | 0.59 | 1.75 | 6 | 2 |
| 1:A:655:ASN:O | 1:A:656:VAL:O | 0.59 | 2.21 | 12 | 16 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:594:ILE:HG23 | 1:A:601:PHE:CG | 0.59 | 2.33 | 3 | 10 |
| 1:A:622:HIS:HD2 | 1:A:680:ILE:HG23 | 0.59 | 1.57 | 18 | 3 |
| 1:A:587:ILE:HD13 | 1:A:688:PHE:CZ | 0.58 | 2.33 | 10 | 8 |
| 1:A:663:ARG:O | 1:A:716:VAL:HG21 | 0.58 | 1.97 | 3 | 6 |
| 1:A:598:VAL:HG11 | 1:A:610:ASN:ND2 | 0.58 | 2.14 | 15 | 1 |
| 1:A:592:LEU:CD2 | 1:A:613:ILE:HD11 | 0.58 | 2.24 | 7 | 1 |
| 1:A:723:GLU:HA | 1:A:726:LEU:HD12 | 0.58 | 1.74 | 17 | 12 |
| 1:A:615:ASP:HB3 | 1:A:618:LEU:HD13 | 0.58 | 1.76 | 14 | 2 |
| 1:A:681:ILE:HG22 | 1:A:690:ILE:CG1 | 0.58 | 2.29 | 10 | 4 |
| 1:A:591:SER:C | 1:A:592:LEU:HD13 | 0.58 | 2.19 | 10 | 3 |
| 1:A:618:LEU:HB2 | 1:A:622:HIS:CG | 0.57 | 2.33 | 17 | 13 |
| 1:A:668:THR:HG22 | 1:A:718:LYS:HA | 0.57 | 1.75 | 20 | 2 |
| 1:A:659:LEU:C | 1:A:659:LEU:HD12 | 0.57 | 2.20 | 17 | 16 |
| 1:A:580:LEU:HD12 | 1:A:594:ILE:CD1 | 0.57 | 2.29 | 20 | 7 |
| 1:A:601:PHE:CZ | 1:A:610:ASN:HB3 | 0.57 | 2.34 | 2 | 18 |
| 1:A:647:ILE:HD12 | 1:A:672:LEU:HB3 | 0.57 | 1.76 | 3 | 6 |
| 1:A:659:LEU:HA | 1:A:678:ILE:HG23 | 0.57 | 1.76 | 10 | 1 |
| 1:A:603:ILE:HD11 | 1:A:625:ILE:HD12 | 0.57 | 1.76 | 14 | 4 |
| 1:A:617:ARG:HB3 | 1:A:681:ILE:HD11 | 0.56 | 1.75 | 10 | 6 |
| 1:A:580:LEU:N | 1:A:592:LEU:O | 0.56 | 2.37 | 7 | 19 |
| 1:A:594:ILE:HG23 | 1:A:601:PHE:CD2 | 0.56 | 2.34 | 1 | 3 |
| 1:A:580:LEU:HD11 | 1:A:625:ILE:HD13 | 0.56 | 1.77 | 15 | 1 |
| 1:A:603:ILE:CG1 | 1:A:611:CYS:HB3 | 0.56 | 2.31 | 14 | 10 |
| 1:A:665:ILE:HG13 | 1:A:668:THR:HG23 | 0.56 | 1.77 | 13 | 1 |
| 1:A:577:PHE:HE1 | 1:A:647:ILE:HG21 | 0.56 | 1.61 | 16 | 5 |
| 1:A:594:ILE:HD11 | 1:A:625:ILE:HD13 | 0.56 | 1.78 | 18 | 2 |
| 1:A:577:PHE:HZ | 1:A:647:ILE:HG21 | 0.56 | 1.58 | 19 | 2 |
| 1:A:649:TYR:CB | 1:A:672:LEU:HD21 | 0.55 | 2.31 | 17 | 10 |
| 1:A:579:THR:HG22 | 1:A:581:LYS:HG3 | 0.55 | 1.77 | 3 | 1 |
| 1:A:578:LEU:CD1 | 1:A:647:ILE:HD13 | 0.55 | 2.26 | 3 | 5 |
| 1:A:648:TRP:CH2 | 1:A:671:LEU:CD2 | 0.55 | 2.89 | 18 | 14 |
| 1:A:649:TYR:HH | 1:A:657:SER:CB | 0.55 | 2.14 | 17 | 2 |
| 1:A:649:TYR:CE2 | 1:A:678:ILE:HD12 | 0.55 | 2.36 | 9 | 1 |
| 1:A:659:LEU:HD11 | 1:A:672:LEU:CD2 | 0.55 | 2.32 | 4 | 1 |
| 1:A:662:ASN:CG | 1:A:716:VAL:HG23 | 0.55 | 2.21 | 18 | 3 |
| 1:A:577:PHE:CD1 | 1:A:577:PHE:C | 0.55 | 2.81 | 15 | 3 |
| 1:A:659:LEU:HD13 | 1:A:678:ILE:HG12 | 0.54 | 1.79 | 2 | 9 |
| 1:A:630:HIS:N | 1:A:644:LEU:O | 0.54 | 2.41 | 5 | 19 |
| 1:A:655:ASN:O | 1:A:656:VAL:HG13 | 0.54 | 2.01 | 10 | 16 |
| 1:A:577:PHE:HB3 | 1:A:596:GLN:HA | 0.54 | 1.77 | 7 | 1 |
| 1:A:602:PHE:CD2 | 1:A:624:PHE:CE1 | 0.54 | 2.96 | 17 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:621:VAL:HG13 | 1:A:621:VAL:O | 0.54 | 2.02 | 11 | 3 |
| 1:A:578:LEU:HD23 | 1:A:578:LEU:C | 0.54 | 2.23 | 18 | 6 |
| 1:A:583:LEU:HD22 | 1:A:693:LYS:HB2 | 0.54 | 1.79 | 10 | 6 |
| 1:A:578:LEU:HD23 | 1:A:594:ILE:CD1 | 0.54 | 2.30 | 7 | 1 |
| 1:A:577:PHE:CD2 | 1:A:698:ASP:O | 0.54 | 2.61 | 7 | 11 |
| 1:A:615:ASP:HB2 | 1:A:618:LEU:HD21 | 0.54 | 1.78 | 16 | 2 |
| 1:A:580:LEU:O | 1:A:592:LEU:N | 0.53 | 2.39 | 18 | 9 |
| 1:A:600:PRO:HG2 | 1:A:602:PHE:CZ | 0.53 | 2.38 | 7 | 14 |
| 1:A:594:ILE:CD1 | 1:A:625:ILE:HG21 | 0.53 | 2.33 | 17 | 2 |
| 1:A:659:LEU:HG | 1:A:678:ILE:HG23 | 0.53 | 1.79 | 18 | 1 |
| 1:A:578:LEU:HD23 | 1:A:579:THR:H | 0.53 | 1.63 | 16 | 1 |
| 1:A:618:LEU:HD12 | 1:A:622:HIS:CG | 0.53 | 2.38 | 2 | 1 |
| 1:A:669:LYS:O | 1:A:717:LEU:HD12 | 0.53 | 2.04 | 13 | 1 |
| 1:A:644:LEU:N | 1:A:644:LEU:CD2 | 0.53 | 2.72 | 4 | 5 |
| 1:A:594:ILE:HG12 | 1:A:601:PHE:CD2 | 0.52 | 2.39 | 5 | 10 |
| 1:A:625:ILE:HG23 | 1:A:648:TRP:O | 0.52 | 2.04 | 5 | 3 |
| 1:A:659:LEU:HD22 | 1:A:678:ILE:HG12 | 0.52 | 1.80 | 19 | 4 |
| 1:A:618:LEU:HD22 | 1:A:680:ILE:HG21 | 0.52 | 1.81 | 9 | 1 |
| 1:A:662:ASN:CB | 1:A:670:PHE:CE2 | 0.52 | 2.93 | 14 | 5 |
| 1:A:655:ASN:C | 1:A:656:VAL:HG13 | 0.52 | 2.25 | 18 | 5 |
| 1:A:579:THR:HG21 | 1:A:581:LYS:CE | 0.52 | 2.35 | 13 | 1 |
| 1:A:577:PHE:HB2 | 1:A:596:GLN:HB3 | 0.52 | 1.82 | 17 | 10 |
| 1:A:656:VAL:HG13 | 1:A:664:MET:O | 0.52 | 2.04 | 4 | 3 |
| 1:A:594:ILE:HG23 | 1:A:601:PHE:HB2 | 0.52 | 1.82 | 12 | 3 |
| 1:A:624:PHE:N | 1:A:650:CYS:O | 0.52 | 2.39 | 17 | 1 |
| 1:A:578:LEU:CD2 | 1:A:694:VAL:HG13 | 0.52 | 2.19 | 16 | 2 |
| 1:A:618:LEU:CB | 1:A:622:HIS:CG | 0.52 | 2.92 | 11 | 9 |
| 1:A:676:ASP:O | 1:A:694:VAL:HB | 0.52 | 2.05 | 17 | 1 |
| 1:A:618:LEU:CB | 1:A:622:HIS:ND1 | 0.51 | 2.72 | 8 | 14 |
| 1:A:578:LEU:CD2 | 1:A:594:ILE:HD12 | 0.51 | 2.32 | 7 | 1 |
| 1:A:577:PHE:CG | 1:A:578:LEU:N | 0.51 | 2.79 | 13 | 7 |
| 1:A:592:LEU:HD22 | 1:A:592:LEU:N | 0.51 | 2.20 | 8 | 4 |
| 1:A:659:LEU:HD23 | 1:A:670:PHE:CD2 | 0.51 | 2.40 | 5 | 1 |
| 1:A:588:ILE:CD1 | 1:A:613:ILE:HG23 | 0.51 | 2.35 | 10 | 7 |
| 1:A:618:LEU:HB3 | 1:A:622:HIS:CE1 | 0.51 | 2.40 | 17 | 1 |
| 1:A:577:PHE:CD1 | 1:A:578:LEU:HB2 | 0.51 | 2.40 | 16 | 4 |
| 1:A:579:THR:O | 1:A:695:GLU:N | 0.51 | 2.42 | 7 | 13 |
| 1:A:594:ILE:HG23 | 1:A:601:PHE:CB | 0.51 | 2.36 | 12 | 3 |
| 1:A:577:PHE:CZ | 1:A:578:LEU:HB2 | 0.51 | 2.41 | 19 | 1 |
| 1:A:627:LYS:HB2 | 1:A:647:ILE:HG22 | 0.51 | 1.82 | 19 | 1 |
| 1:A:582:PRO:CD | 1:A:592:LEU:HD22 | 0.50 | 2.36 | 11 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:627:LYS:CE | 1:A:647:ILE:HG23 | 0.50 | 2.35 | 5 | 1 |
| 1:A:583:LEU:H | 1:A:583:LEU:HD13 | 0.50 | 1.66 | 18 | 3 |
| 1:A:578:LEU:CG | 1:A:694:VAL:HG13 | 0.50 | 2.36 | 6 | 6 |
| 1:A:649:TYR:HB2 | 1:A:672:LEU:HD11 | 0.50 | 1.83 | 19 | 4 |
| 1:A:577:PHE:HB3 | 1:A:596:GLN:CA | 0.50 | 2.37 | 7 | 1 |
| 1:A:615:ASP:HB3 | 1:A:618:LEU:CD1 | 0.50 | 2.36 | 14 | 2 |
| 1:A:582:PRO:CD | 1:A:590:GLU:O | 0.50 | 2.59 | 10 | 20 |
| 1:A:595:GLN:O | 1:A:596:GLN:C | 0.50 | 2.49 | 6 | 2 |
| 1:A:587:ILE:HG22 | 1:A:689:VAL:O | 0.50 | 2.07 | 14 | 1 |
| 1:A:577:PHE:CD1 | 1:A:578:LEU:N | 0.50 | 2.79 | 16 | 2 |
| 1:A:648:TRP:CZ3 | 1:A:671:LEU:HG | 0.50 | 2.41 | 1 | 5 |
| 1:A:716:VAL:HG13 | 1:A:716:VAL:O | 0.50 | 2.07 | 1 | 4 |
| 1:A:580:LEU:HD23 | 1:A:694:VAL:CG2 | 0.50 | 2.37 | 6 | 1 |
| 1:A:662:ASN:HB3 | 1:A:716:VAL:HG23 | 0.50 | 1.83 | 12 | 1 |
| 1:A:592:LEU:HD11 | 1:A:692:PHE:CD2 | 0.49 | 2.41 | 17 | 3 |
| 1:A:595:GLN:O | 1:A:597:GLY:N | 0.49 | 2.45 | 6 | 1 |
| 1:A:618:LEU:HD23 | 1:A:680:ILE:CG2 | 0.49 | 2.37 | 5 | 6 |
| 1:A:656:VAL:HG23 | 1:A:664:MET:O | 0.49 | 2.07 | 2 | 3 |
| 1:A:659:LEU:HD12 | 1:A:660:ASN:N | 0.49 | 2.23 | 9 | 2 |
| 1:A:659:LEU:CD2 | 1:A:678:ILE:HG22 | 0.49 | 2.33 | 11 | 1 |
| 1:A:584:PRO:HA | 1:A:589:GLN:CD | 0.49 | 2.28 | 5 | 3 |
| 1:A:584:PRO:O | 1:A:589:GLN:NE2 | 0.49 | 2.45 | 7 | 3 |
| 1:A:580:LEU:HD21 | 1:A:625:ILE:CD1 | 0.49 | 2.37 | 6 | 1 |
| 1:A:648:TRP:CZ3 | 1:A:717:LEU:HD12 | 0.49 | 2.42 | 10 | 1 |
| 1:A:649:TYR:HB3 | 1:A:672:LEU:HD21 | 0.49 | 1.83 | 17 | 1 |
| 1:A:648:TRP:CZ2 | 1:A:671:LEU:HD22 | 0.49 | 2.42 | 2 | 1 |
| 1:A:587:ILE:CD1 | 1:A:688:PHE:CZ | 0.49 | 2.95 | 7 | 11 |
| 1:A:651:HIS:CE1 | 1:A:657:SER:HG | 0.49 | 2.26 | 16 | 1 |
| 1:A:615:ASP:OD2 | 1:A:681:ILE:HG21 | 0.49 | 2.07 | 3 | 5 |
| 1:A:578:LEU:C | 1:A:578:LEU:HD23 | 0.48 | 2.27 | 3 | 3 |
| 1:A:652:THR:O | 1:A:666:GLN:NE2 | 0.48 | 2.46 | 16 | 4 |
| 1:A:578:LEU:CD1 | 1:A:647:ILE:CD1 | 0.48 | 2.91 | 9 | 5 |
| 1:A:651:HIS:CG | 1:A:657:SER:HG | 0.48 | 2.26 | 4 | 1 |
| 1:A:627:LYS:HD3 | 1:A:647:ILE:HG23 | 0.48 | 1.85 | 20 | 2 |
| 1:A:659:LEU:HD13 | 1:A:678:ILE:CG2 | 0.48 | 2.31 | 15 | 2 |
| 1:A:659:LEU:CD1 | 1:A:670:PHE:CD2 | 0.48 | 2.97 | 18 | 1 |
| 1:A:577:PHE:CB | 1:A:596:GLN:HB3 | 0.48 | 2.38 | 3 | 11 |
| 1:A:682:TRP:CD1 | 1:A:689:VAL:HG13 | 0.48 | 2.42 | 4 | 1 |
| 1:A:622:HIS:CD2 | 1:A:680:ILE:CG2 | 0.48 | 2.96 | 15 | 3 |
| 1:A:587:ILE:HG12 | 1:A:690:ILE:HD11 | 0.48 | 1.84 | 9 | 1 |
| 1:A:659:LEU:O | 1:A:661:ASN:N | 0.48 | 2.47 | 9 | 14 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:587:ILE:CD1 | 1:A:688:PHE:CE1 | 0.48 | 2.97 | 11 | 3 |
| 1:A:579:THR:HG22 | 1:A:581:LYS:HG2 | 0.47 | 1.86 | 11 | 1 |
| 1:A:578:LEU:HD13 | 1:A:696:ILE:HG12 | 0.47 | 1.86 | 1 | 1 |
| 1:A:675:GLY:N | 1:A:694:VAL:O | 0.47 | 2.47 | 6 | 16 |
| 1:A:659:LEU:CD1 | 1:A:678:ILE:HG22 | 0.47 | 2.32 | 15 | 1 |
| 1:A:583:LEU:HD12 | 1:A:585:ASP:CB | 0.47 | 2.39 | 15 | 2 |
| 1:A:662:ASN:CB | 1:A:670:PHE:CE1 | 0.47 | 2.97 | 13 | 2 |
| 1:A:617:ARG:HB3 | 1:A:681:ILE:HD13 | 0.47 | 1.85 | 14 | 1 |
| 1:A:658:TYR:O | 1:A:679:LYS:N | 0.47 | 2.43 | 8 | 3 |
| 1:A:644:LEU:HD12 | 1:A:644:LEU:N | 0.47 | 2.25 | 6 | 2 |
| 1:A:692:PHE:N | 1:A:692:PHE:CD1 | 0.47 | 2.81 | 19 | 4 |
| 1:A:605:ARG:CG | 1:A:618:LEU:HD12 | 0.47 | 2.40 | 16 | 1 |
| 1:A:578:LEU:HD12 | 1:A:579:THR:N | 0.47 | 2.23 | 17 | 1 |
| 1:A:662:ASN:HB2 | 1:A:670:PHE:CE2 | 0.47 | 2.45 | 2 | 4 |
| 1:A:582:PRO:CB | 1:A:588:ILE:HG23 | 0.47 | 2.40 | 19 | 2 |
| 1:A:577:PHE:HB2 | 1:A:596:GLN:HA | 0.47 | 1.86 | 7 | 1 |
| 1:A:592:LEU:HD11 | 1:A:692:PHE:CE2 | 0.47 | 2.44 | 18 | 2 |
| 1:A:580:LEU:HB3 | 1:A:592:LEU:HD12 | 0.47 | 1.87 | 19 | 1 |
| 1:A:592:LEU:CD1 | 1:A:692:PHE:CD2 | 0.47 | 2.98 | 17 | 4 |
| 1:A:649:TYR:O | 1:A:669:LYS:HA | 0.47 | 2.10 | 20 | 3 |
| 1:A:618:LEU:HD12 | 1:A:622:HIS:CB | 0.47 | 2.40 | 15 | 1 |
| 1:A:577:PHE:CE2 | 1:A:578:LEU:HB2 | 0.46 | 2.44 | 13 | 3 |
| 1:A:615:ASP:CB | 1:A:618:LEU:HD21 | 0.46 | 2.40 | 16 | 2 |
| 1:A:671:LEU:HD12 | 1:A:672:LEU:N | 0.46 | 2.25 | 2 | 1 |
| 1:A:583:LEU:HD22 | 1:A:583:LEU:N | 0.46 | 2.25 | 19 | 3 |
| 1:A:621:VAL:HG12 | 1:A:621:VAL:O | 0.46 | 2.10 | 9 | 1 |
| 1:A:587:ILE:CG2 | 1:A:690:ILE:HD13 | 0.46 | 2.41 | 10 | 1 |
| 1:A:580:LEU:CD1 | 1:A:594:ILE:CD1 | 0.46 | 2.94 | 14 | 3 |
| 1:A:578:LEU:O | 1:A:594:ILE:N | 0.46 | 2.48 | 4 | 7 |
| 1:A:594:ILE:HG12 | 1:A:601:PHE:CD1 | 0.46 | 2.46 | 9 | 2 |
| 1:A:681:ILE:HG22 | 1:A:690:ILE:CB | 0.46 | 2.35 | 12 | 1 |
| 1:A:651:HIS:CE1 | 1:A:657:SER:N | 0.46 | 2.84 | 15 | 13 |
| 1:A:617:ARG:CB | 1:A:681:ILE:CD1 | 0.46 | 2.94 | 8 | 4 |
| 1:A:583:LEU:HD21 | 1:A:677:GLU:HG3 | 0.46 | 1.87 | 17 | 1 |
| 1:A:655:ASN:O | 1:A:656:VAL:CG1 | 0.46 | 2.64 | 2 | 2 |
| 1:A:681:ILE:HG22 | 1:A:690:ILE:HG13 | 0.46 | 1.88 | 10 | 2 |
| 1:A:577:PHE:CD1 | 1:A:696:ILE:HG23 | 0.46 | 2.46 | 20 | 1 |
| 1:A:602:PHE:HA | 1:A:624:PHE:CB | 0.46 | 2.41 | 15 | 10 |
| 1:A:615:ASP:OD1 | 1:A:688:PHE:CZ | 0.46 | 2.68 | 9 | 5 |
| 1:A:577:PHE:CE1 | 1:A:647:ILE:CG2 | 0.45 | 2.99 | 9 | 6 |
| 1:A:655:ASN:C | 1:A:656:VAL:CG1 | 0.45 | 2.85 | 10 | 16 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:659:LEU:HD21 | 1:A:672:LEU:HD22 | 0.45 | 1.88 | 19 | 3 |
| 1:A:617:ARG:O | 1:A:655:ASN:ND2 | 0.45 | 2.48 | 7 | 3 |
| 1:A:605:ARG:HG2 | 1:A:618:LEU:CD1 | 0.45 | 2.41 | 6 | 11 |
| 1:A:579:THR:HG22 | 1:A:581:LYS:CG | 0.45 | 2.41 | 3 | 3 |
| 1:A:618:LEU:HB2 | 1:A:622:HIS:ND1 | 0.45 | 2.25 | 9 | 2 |
| 1:A:681:ILE:CG2 | 1:A:690:ILE:HD12 | 0.45 | 2.41 | 14 | 1 |
| 1:A:648:TRP:CH2 | 1:A:671:LEU:HG | 0.45 | 2.47 | 10 | 5 |
| 1:A:579:THR:HG21 | 1:A:581:LYS:HE2 | 0.45 | 1.88 | 13 | 1 |
| 1:A:600:PRO:HB2 | 1:A:624:PHE:CE1 | 0.45 | 2.47 | 16 | 2 |
| 1:A:589:GLN:OE1 | 1:A:589:GLN:CA | 0.45 | 2.64 | 5 | 3 |
| 1:A:587:ILE:CG2 | 1:A:690:ILE:CD1 | 0.45 | 2.95 | 10 | 1 |
| 1:A:587:ILE:HG21 | 1:A:688:PHE:CE1 | 0.45 | 2.45 | 2 | 1 |
| 1:A:587:ILE:HG23 | 1:A:588:ILE:HG13 | 0.45 | 1.89 | 14 | 1 |
| 1:A:615:ASP:H | 1:A:618:LEU:HD11 | 0.45 | 1.72 | 7 | 8 |
| 1:A:670:PHE:CE1 | 1:A:716:VAL:HG22 | 0.45 | 2.46 | 6 | 2 |
| 1:A:627:LYS:HB3 | 1:A:647:ILE:HG22 | 0.45 | 1.89 | 13 | 1 |
| 1:A:618:LEU:HD12 | 1:A:622:HIS:CD2 | 0.45 | 2.47 | 2 | 1 |
| 1:A:580:LEU:N | 1:A:580:LEU:HD23 | 0.45 | 2.26 | 7 | 1 |
| 1:A:603:ILE:HG13 | 1:A:611:CYS:HB3 | 0.45 | 1.88 | 18 | 4 |
| 1:A:689:VAL:CG1 | 1:A:689:VAL:O | 0.45 | 2.64 | 12 | 1 |
| 1:A:580:LEU:HD11 | 1:A:594:ILE:CD1 | 0.45 | 2.42 | 16 | 1 |
| 1:A:594:ILE:CD1 | 1:A:625:ILE:HD13 | 0.45 | 2.42 | 18 | 1 |
| 1:A:618:LEU:HD23 | 1:A:618:LEU:C | 0.45 | 2.31 | 2 | 1 |
| 1:A:582:PRO:HB3 | 1:A:588:ILE:CG2 | 0.45 | 2.42 | 3 | 1 |
| 1:A:612:LYS:O | 1:A:613:ILE:HD13 | 0.45 | 2.11 | 20 | 2 |
| 1:A:699:THR:O | 1:A:699:THR:OG1 | 0.45 | 2.35 | 12 | 5 |
| 1:A:662:ASN:ND2 | 1:A:716:VAL:HG23 | 0.44 | 2.27 | 6 | 2 |
| 1:A:648:TRP:HB3 | 1:A:669:LYS:CG | 0.44 | 2.42 | 13 | 2 |
| 1:A:662:ASN:HB3 | 1:A:670:PHE:CE2 | 0.44 | 2.47 | 14 | 1 |
| 1:A:577:PHE:CE1 | 1:A:696:ILE:HG23 | 0.44 | 2.47 | 3 | 1 |
| 1:A:615:ASP:HB3 | 1:A:618:LEU:CD2 | 0.44 | 2.40 | 10 | 4 |
| 1:A:592:LEU:HD13 | 1:A:592:LEU:N | 0.44 | 2.26 | 10 | 1 |
| 1:A:583:LEU:HD22 | 1:A:583:LEU:H | 0.44 | 1.72 | 19 | 1 |
| 1:A:651:HIS:ND1 | 1:A:657:SER:OG | 0.44 | 2.51 | 17 | 4 |
| 1:A:578:LEU:HD12 | 1:A:696:ILE:CG1 | 0.44 | 2.42 | 2 | 2 |
| 1:A:603:ILE:CD1 | 1:A:625:ILE:CD1 | 0.44 | 2.96 | 4 | 3 |
| 1:A:627:LYS:HA | 1:A:646:ASP:O | 0.44 | 2.13 | 13 | 1 |
| 1:A:583:LEU:HD12 | 1:A:585:ASP:HB3 | 0.44 | 1.89 | 15 | 1 |
| 1:A:615:ASP:OD2 | 1:A:688:PHE:CE1 | 0.44 | 2.71 | 11 | 3 |
| 1:A:724:LYS:O | 1:A:727:VAL:HG12 | 0.44 | 2.12 | 6 | 2 |
| 1:A:678:ILE:CD1 | 1:A:694:VAL:HG23 | 0.44 | 2.42 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:580:LEU:HD22 | 1:A:692:PHE:HB2 | 0.44 | 1.88 | 1 | 2 |
| 1:A:594:ILE:CD1 | 1:A:625:ILE:CD1 | 0.44 | 2.94 | 8 | 4 |
| 1:A:654:THR:HG23 | 1:A:655:ASN:N | 0.44 | 2.27 | 1 | 2 |
| 1:A:659:LEU:HD11 | 1:A:676:ASP:OD1 | 0.44 | 2.13 | 9 | 3 |
| 1:A:655:ASN:CB | 1:A:681:ILE:HD12 | 0.44 | 2.43 | 4 | 2 |
| 1:A:626:PHE:CE1 | 1:A:627:LYS:O | 0.44 | 2.71 | 6 | 16 |
| 1:A:601:PHE:CE2 | 1:A:610:ASN:HB3 | 0.44 | 2.47 | 5 | 3 |
| 1:A:655:ASN:HB3 | 1:A:681:ILE:HD12 | 0.44 | 1.90 | 14 | 2 |
| 1:A:648:TRP:CZ3 | 1:A:717:LEU:CD1 | 0.44 | 3.01 | 7 | 2 |
| 1:A:577:PHE:CZ | 1:A:647:ILE:CG2 | 0.44 | 3.01 | 11 | 1 |
| 1:A:600:PRO:CG | 1:A:624:PHE:CZ | 0.44 | 3.00 | 16 | 1 |
| 1:A:626:PHE:CZ | 1:A:628:LYS:CG | 0.44 | 3.01 | 2 | 8 |
| 1:A:659:LEU:HD12 | 1:A:670:PHE:HB3 | 0.43 | 1.89 | 4 | 1 |
| 1:A:615:ASP:OD1 | 1:A:690:ILE:HD11 | 0.43 | 2.13 | 12 | 1 |
| 1:A:669:LYS:O | 1:A:717:LEU:N | 0.43 | 2.51 | 16 | 1 |
| 1:A:676:ASP:OD1 | 1:A:678:ILE:HG23 | 0.43 | 2.13 | 17 | 1 |
| 1:A:617:ARG:NH1 | 1:A:688:PHE:CE1 | 0.43 | 2.86 | 19 | 1 |
| 1:A:618:LEU:CD2 | 1:A:680:ILE:CG2 | 0.43 | 2.96 | 5 | 2 |
| 1:A:659:LEU:CD2 | 1:A:672:LEU:CD2 | 0.43 | 2.97 | 1 | 2 |
| 1:A:689:VAL:O | 1:A:689:VAL:CG1 | 0.43 | 2.65 | 5 | 12 |
| 1:A:651:HIS:ND1 | 1:A:657:SER:CB | 0.43 | 2.81 | 10 | 4 |
| 1:A:681:ILE:CG2 | 1:A:690:ILE:HB | 0.43 | 2.43 | 9 | 1 |
| 1:A:577:PHE:CE1 | 1:A:578:LEU:HB2 | 0.43 | 2.48 | 19 | 1 |
| 1:A:617:ARG:NH1 | 1:A:688:PHE:CD2 | 0.43 | 2.86 | 2 | 1 |
| 1:A:617:ARG:HB3 | 1:A:681:ILE:CD1 | 0.43 | 2.43 | 19 | 3 |
| 1:A:576:ARG:O | 1:A:698:ASP:CB | 0.43 | 2.66 | 11 | 4 |
| 1:A:615:ASP:HB3 | 1:A:618:LEU:HG | 0.43 | 1.90 | 11 | 1 |
| 1:A:604:GLY:HA3 | 1:A:620:ARG:O | 0.43 | 2.12 | 1 | 5 |
| 1:A:629:ARG:O | 1:A:629:ARG:HG3 | 0.43 | 2.14 | 9 | 3 |
| 1:A:578:LEU:HD23 | 1:A:580:LEU:HD21 | 0.43 | 1.90 | 10 | 1 |
| 1:A:583:LEU:HD22 | 1:A:691:GLY:O | 0.43 | 2.13 | 18 | 1 |
| 1:A:655:ASN:C | 1:A:656:VAL:HG23 | 0.43 | 2.33 | 16 | 2 |
| 1:A:582:PRO:CD | 1:A:592:LEU:CD2 | 0.43 | 2.96 | 9 | 6 |
| 1:A:615:ASP:CB | 1:A:618:LEU:CD2 | 0.43 | 2.96 | 11 | 2 |
| 1:A:681:ILE:O | 1:A:690:ILE:N | 0.43 | 2.50 | 15 | 1 |
| 1:A:622:HIS:NE2 | 1:A:680:ILE:HG23 | 0.43 | 2.28 | 19 | 1 |
| 1:A:580:LEU:CD2 | 1:A:694:VAL:CG2 | 0.43 | 2.96 | 8 | 3 |
| 1:A:600:PRO:HB3 | 1:A:626:PHE:HB2 | 0.43 | 1.91 | 11 | 8 |
| 1:A:617:ARG:NH1 | 1:A:688:PHE:CE2 | 0.43 | 2.87 | 2 | 1 |
| 1:A:595:GLN:CB | 1:A:598:VAL:HG23 | 0.43 | 2.43 | 16 | 1 |
| 1:A:690:ILE:CG2 | 1:A:691:GLY:N | 0.43 | 2.82 | 11 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:670:PHE:CD1 | 1:A:671:LEU:N | 0.43 | 2.87 | 11 | 1 |
| 1:A:577:PHE:HB3 | 1:A:596:GLN:HB3 | 0.43 | 1.91 | 19 | 1 |
| 1:A:651:HIS:ND1 | 1:A:657:SER:HB3 | 0.42 | 2.29 | 3 | 2 |
| 1:A:692:PHE:CD1 | 1:A:692:PHE:N | 0.42 | 2.85 | 6 | 3 |
| 1:A:648:TRP:CZ3 | 1:A:717:LEU:HD11 | 0.42 | 2.48 | 7 | 1 |
| 1:A:577:PHE:HE1 | 1:A:647:ILE:HD13 | 0.42 | 1.74 | 9 | 1 |
| 1:A:587:ILE:HG21 | 1:A:688:PHE:CZ | 0.42 | 2.49 | 3 | 1 |
| 1:A:618:LEU:CD2 | 1:A:680:ILE:HG21 | 0.42 | 2.44 | 3 | 1 |
| 1:A:620:ARG:CG | 1:A:621:VAL:HG23 | 0.42 | 2.44 | 3 | 2 |
| 1:A:659:LEU:C | 1:A:659:LEU:CD1 | 0.42 | 2.87 | 17 | 2 |
| 1:A:617:ARG:NH1 | 1:A:688:PHE:CZ | 0.42 | 2.87 | 19 | 1 |
| 1:A:605:ARG:NE | 1:A:618:LEU:O | 0.42 | 2.53 | 10 | 5 |
| 1:A:576:ARG:CG | 1:A:593:GLU:CB | 0.42 | 2.97 | 4 | 1 |
| 1:A:656:VAL:CG1 | 1:A:664:MET:O | 0.42 | 2.67 | 4 | 1 |
| 1:A:615:ASP:OD2 | 1:A:688:PHE:CZ | 0.42 | 2.72 | 11 | 1 |
| 1:A:587:ILE:CD1 | 1:A:690:ILE:CG1 | 0.42 | 2.97 | 18 | 1 |
| 1:A:656:VAL:HG22 | 1:A:658:TYR:CZ | 0.42 | 2.49 | 18 | 1 |
| 1:A:586:SER:OG | 1:A:690:ILE:HA | 0.42 | 2.14 | 5 | 1 |
| 1:A:659:LEU:HG | 1:A:670:PHE:CD2 | 0.42 | 2.49 | 9 | 5 |
| 1:A:674:ASP:HB3 | 1:A:696:ILE:HD12 | 0.42 | 1.91 | 2 | 1 |
| 1:A:596:GLN:HG2 | 1:A:597:GLY:N | 0.42 | 2.29 | 10 | 2 |
| 1:A:664:MET:HE1 | 1:A:670:PHE:HB2 | 0.42 | 1.91 | 13 | 2 |
| 1:A:582:PRO:HB2 | 1:A:588:ILE:HG23 | 0.42 | 1.92 | 3 | 1 |
| 1:A:670:PHE:CD1 | 1:A:716:VAL:HG22 | 0.42 | 2.50 | 13 | 1 |
| 1:A:583:LEU:HD12 | 1:A:693:LYS:CB | 0.42 | 2.41 | 18 | 1 |
| 1:A:615:ASP:HB2 | 1:A:618:LEU:HD13 | 0.42 | 1.89 | 19 | 1 |
| 1:A:578:LEU:CD1 | 1:A:696:ILE:HG12 | 0.42 | 2.45 | 2 | 2 |
| 1:A:626:PHE:CZ | 1:A:628:LYS:HG3 | 0.42 | 2.49 | 10 | 4 |
| 1:A:659:LEU:CG | 1:A:678:ILE:HG22 | 0.42 | 2.42 | 4 | 1 |
| 1:A:651:HIS:CE1 | 1:A:657:SER:OG | 0.42 | 2.72 | 16 | 3 |
| 1:A:662:ASN:ND2 | 1:A:670:PHE:CE2 | 0.42 | 2.88 | 8 | 1 |
| 1:A:598:VAL:HG11 | 1:A:610:ASN:CG | 0.42 | 2.35 | 18 | 3 |
| 1:A:592:LEU:HD13 | 1:A:611:CYS:HG | 0.42 | 1.72 | 18 | 1 |
| 1:A:577:PHE:CB | 1:A:596:GLN:HG2 | 0.42 | 2.45 | 4 | 2 |
| 1:A:578:LEU:CD1 | 1:A:696:ILE:CG1 | 0.42 | 2.97 | 2 | 3 |
| 1:A:578:LEU:HD21 | 1:A:694:VAL:CG2 | 0.41 | 2.45 | 8 | 1 |
| 1:A:674:ASP:N | 1:A:696:ILE:HD12 | 0.41 | 2.29 | 8 | 1 |
| 1:A:659:LEU:CA | 1:A:678:ILE:HG23 | 0.41 | 2.44 | 10 | 1 |
| 1:A:649:TYR:CD2 | 1:A:664:MET:CE | 0.41 | 3.04 | 4 | 1 |
| 1:A:580:LEU:HD11 | 1:A:625:ILE:HD12 | 0.41 | 1.92 | 10 | 1 |
| 1:A:618:LEU:HD23 | 1:A:680:ILE:HG23 | 0.41 | 1.91 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:618:LEU:HG | 1:A:622:HIS:CG | 0.41 | 2.50 | 14 | 1 |
| 1:A:647:ILE:HD11 | 1:A:672:LEU:O | 0.41 | 2.16 | 9 | 1 |
| 1:A:624:PHE:O | 1:A:650:CYS:HB2 | 0.41 | 2.15 | 10 | 1 |
| 1:A:675:GLY:CA | 1:A:694:VAL:O | 0.41 | 2.68 | 10 | 1 |
| 1:A:658:TYR:N | 1:A:679:LYS:O | 0.41 | 2.46 | 16 | 1 |
| 1:A:651:HIS:CE1 | 1:A:657:SER:HB3 | 0.41 | 2.51 | 1 | 2 |
| 1:A:587:ILE:N | 1:A:689:VAL:O | 0.41 | 2.49 | 3 | 1 |
| 1:A:581:LYS:HA | 1:A:591:SER:HA | 0.41 | 1.91 | 2 | 1 |
| 1:A:588:ILE:HD12 | 1:A:690:ILE:HD13 | 0.41 | 1.93 | 5 | 1 |
| 1:A:630:HIS:CD2 | 1:A:630:HIS:C | 0.41 | 2.93 | 11 | 1 |
| 1:A:580:LEU:HD12 | 1:A:594:ILE:HG13 | 0.41 | 1.92 | 16 | 1 |
| 1:A:626:PHE:CE2 | 1:A:627:LYS:O | 0.41 | 2.73 | 16 | 1 |
| 1:A:587:ILE:HD13 | 1:A:587:ILE:N | 0.41 | 2.30 | 19 | 1 |
| 1:A:600:PRO:HG2 | 1:A:602:PHE:CE2 | 0.41 | 2.50 | 7 | 1 |
| 1:A:582:PRO:HG3 | 1:A:692:PHE:CE1 | 0.41 | 2.51 | 12 | 2 |
| 1:A:662:ASN:OD1 | 1:A:670:PHE:CZ | 0.41 | 2.74 | 16 | 2 |
| 1:A:659:LEU:HD23 | 1:A:670:PHE:HB3 | 0.41 | 1.92 | 20 | 1 |
| 1:A:685:ASN:ND2 | 1:A:686:ASN:N | 0.41 | 2.69 | 10 | 1 |
| 1:A:657:SER:O | 1:A:664:MET:CB | 0.41 | 2.69 | 16 | 1 |
| 1:A:626:PHE:O | 1:A:648:TRP:N | 0.41 | 2.46 | 2 | 1 |
| 1:A:622:HIS:CD2 | 1:A:680:ILE:O | 0.41 | 2.74 | 4 | 1 |
| 1:A:595:GLN:O | 1:A:598:VAL:HG23 | 0.41 | 2.15 | 7 | 1 |
| 1:A:578:LEU:HD13 | 1:A:696:ILE:CG1 | 0.41 | 2.46 | 12 | 1 |
| 1:A:600:PRO:HG2 | 1:A:602:PHE:CE1 | 0.41 | 2.51 | 13 | 1 |
| 1:A:676:ASP:HB3 | 1:A:694:VAL:HB | 0.41 | 1.93 | 17 | 1 |
| 1:A:603:ILE:HD11 | 1:A:625:ILE:CD1 | 0.41 | 2.45 | 14 | 2 |
| 1:A:662:ASN:HB2 | 1:A:670:PHE:CZ | 0.41 | 2.50 | 6 | 1 |
| 1:A:580:LEU:CD1 | 1:A:625:ILE:HD13 | 0.41 | 2.44 | 15 | 1 |
| 1:A:652:THR:O | 1:A:666:GLN:CG | 0.40 | 2.69 | 14 | 2 |
| 1:A:658:TYR:CD1 | 1:A:658:TYR:N | 0.40 | 2.89 | 12 | 1 |
| 1:A:621:VAL:O | 1:A:652:THR:OG1 | 0.40 | 2.38 | 16 | 1 |
| 1:A:655:ASN:CB | 1:A:681:ILE:CD1 | 0.40 | 2.99 | 4 | 1 |
| 1:A:688:PHE:O | 1:A:688:PHE:CD1 | 0.40 | 2.74 | 4 | 1 |
| 1:A:649:TYR:CE2 | 1:A:678:ILE:HG21 | 0.40 | 2.51 | 7 | 1 |
| 1:A:578:LEU:CD2 | 1:A:647:ILE:CD1 | 0.40 | 2.97 | 10 | 1 |
| 1:A:655:ASN:ND2 | 1:A:681:ILE:HD11 | 0.40 | 2.30 | 17 | 1 |
| 1:A:662:ASN:HB3 | 1:A:716:VAL:CG2 | 0.40 | 2.46 | 12 | 1 |
| 1:A:576:ARG:CG | 1:A:593:GLU:HB3 | 0.40 | 2.46 | 15 | 1 |
| 1:A:615:ASP:HB3 | 1:A:618:LEU:CG | 0.40 | 2.46 | 17 | 1 |
| 1:A:576:ARG:CD | 1:A:593:GLU:HB3 | 0.40 | 2.46 | 6 | 1 |
| 1:A:657:SER:O | 1:A:664:MET:N | 0.40 | 2.53 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:578:LEU:HG | 1:A:694:VAL:HG13 | 0.40 | 1.93 | 19 | 1 |
| 1:A:664:MET:CE | 1:A:670:PHE:HB2 | 0.40 | 2.46 | 20 | 1 |
| 1:A:646:ASP:CG | 1:A:671:LEU:HD11 | 0.40 | 2.37 | 3 | 1 |
| 1:A:618:LEU:HB3 | 1:A:622:HIS:CG | 0.40 | 2.52 | 7 | 1 |
| 1:A:649:TYR:OH | 1:A:657:SER:CB | 0.40 | 2.69 | 11 | 1 |
| 1:A:654:THR:CG2 | 1:A:655:ASN:N | 0.40 | 2.85 | 16 | 1 |
| 1:A:651:HIS:NE2 | 1:A:656:VAL:HA | 0.40 | 2.32 | 20 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 125/158 (79%) | 112±2 (90±2%) | 9±2 (7±1%) | 4±1 (3±1%) | 6 36 |
| 2 | P | 0 | - | - | - | - |
| All | All | 2500/3340 (75%) | 2239 (90%) | 176 (7%) | 85 (3%) | 6 36 |

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 656 | VAL | 20 |
| 1 | A | 660 | ASN | 20 |
| 1 | A | 582 | PRO | 19 |
| 1 | A | 666 | GLN | 15 |
| 1 | A | 616 | ASN | 5 |
| 1 | A | 674 | ASP | 4 |
| 1 | A | 596 | GLN | 1 |
| 1 | A | 619 | SER | 1 |

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation

was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 118/142 (83%) | 85±3 (72±3%) | 33±3 (28±3%) | 2 20 |
| 2 | P | 0 | - | - | - |
| All | All | 2360/3000 (79%) | 1704 (72%) | 656 (28%) | 2 20 |

All 85 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 583 | LEU | 20 |
| 1 | A | 591 | SER | 20 |
| 1 | A | 612 | LYS | 20 |
| 1 | A | 628 | LYS | 20 |
| 1 | A | 659 | LEU | 20 |
| 1 | A | 671 | LEU | 20 |
| 1 | A | 589 | GLN | 19 |
| 1 | A | 596 | GLN | 19 |
| 1 | A | 676 | ASP | 19 |
| 1 | A | 605 | ARG | 18 |
| 1 | A | 606 | SER | 18 |
| 1 | A | 592 | LEU | 16 |
| 1 | A | 616 | ASN | 16 |
| 1 | A | 718 | LYS | 16 |
| 1 | A | 646 | ASP | 15 |
| 1 | A | 656 | VAL | 15 |
| 1 | A | 618 | LEU | 13 |
| 1 | A | 620 | ARG | 13 |
| 1 | A | 670 | PHE | 13 |
| 1 | A | 577 | PHE | 13 |
| 1 | A | 593 | GLU | 12 |
| 1 | A | 580 | LEU | 12 |
| 1 | A | 717 | LEU | 11 |
| 1 | A | 617 | ARG | 11 |
| 1 | A | 629 | ARG | 10 |
| 1 | A | 645 | ASP | 9 |
| 1 | A | 680 | ILE | 9 |
| 1 | A | 695 | GLU | 9 |
| 1 | A | 607 | GLU | 8 |
| 1 | A | 677 | GLU | 8 |
| 1 | A | 687 | LYS | 8 |
| 1 | A | 644 | LEU | 7 |
| 1 | A | 728 | LYS | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 581 | LYS | 7 |
| 1 | A | 693 | LYS | 7 |
| 1 | A | 672 | LEU | 7 |
| 1 | A | 684 | LYS | 7 |
| 1 | A | 686 | ASN | 7 |
| 1 | A | 699 | THR | 7 |
| 1 | A | 679 | LYS | 7 |
| 1 | A | 595 | GLN | 6 |
| 1 | A | 673 | GLN | 6 |
| 1 | A | 585 | ASP | 6 |
| 1 | A | 619 | SER | 6 |
| 1 | A | 689 | VAL | 6 |
| 1 | A | 720 | THR | 6 |
| 1 | A | 697 | ASN | 5 |
| 1 | A | 723 | GLU | 5 |
| 1 | A | 655 | ASN | 5 |
| 1 | A | 662 | ASN | 5 |
| 1 | A | 666 | GLN | 5 |
| 1 | A | 586 | SER | 4 |
| 1 | A | 587 | ILE | 4 |
| 1 | A | 663 | ARG | 4 |
| 1 | A | 614 | GLU | 4 |
| 1 | A | 681 | ILE | 4 |
| 1 | A | 688 | PHE | 4 |
| 1 | A | 608 | ASP | 4 |
| 1 | A | 647 | ILE | 4 |
| 1 | A | 650 | CYS | 3 |
| 1 | A | 668 | THR | 3 |
| 1 | A | 683 | ASP | 3 |
| 1 | A | 576 | ARG | 3 |
| 1 | A | 615 | ASP | 3 |
| 1 | A | 664 | MET | 3 |
| 1 | A | 694 | VAL | 2 |
| 1 | A | 698 | ASP | 2 |
| 1 | A | 610 | ASN | 2 |
| 1 | A | 724 | LYS | 2 |
| 1 | A | 626 | PHE | 2 |
| 1 | A | 661 | ASN | 2 |
| 1 | A | 725 | ASP | 2 |
| 1 | A | 660 | ASN | 2 |
| 1 | A | 722 | GLU | 2 |
| 1 | A | 729 | LYS | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 623 | CYS | 2 |
| 1 | A | 624 | PHE | 2 |
| 1 | A | 627 | LYS | 1 |
| 1 | A | 685 | ASN | 1 |
| 1 | A | 599 | ASN | 1 |
| 1 | A | 678 | ILE | 1 |
| 1 | A | 719 | GLN | 1 |
| 1 | A | 602 | PHE | 1 |
| 1 | A | 669 | LYS | 1 |
| 1 | A | 692 | PHE | 1 |

### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | TPO | P | 603 | 2 | 8,10,11 | 0.96±0.02 | 0±0 (0±0%) |

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

| Mol | Type | Chain | Res | Link | Bond angles | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | TPO | P | 603 | 2 | 10,14,16 | 1.12±0.02 | 0±0 (0±0%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | TPO | P | 603 | 2 | - | 0±0,9,11,13 | - |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

There are no ligands in this entry.

## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

No chemical shift data were provided