

Full wwPDB NMR Structure Validation Report (i)

Dec 19, 2023 – 06:13 PM EST

| PDB ID | : | 1UFM |
|--------------|---|--|
| Title | : | Solution structure of the PCI domain |
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| | | S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI) |
| Deposited on | : | 2003-06-02 |

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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

| Cyrange | : | Kirchner and Güntert (2011) |
|--------------------------------|---|--|
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v 1n 11 5 13 A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

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.



| Ramachandran outliers | 154571 | 11451 | |
|----------------------------|--------------------------|-----------------------|---------------------------------|
| Sidechain outliers | 154315 | 11428 | |
| | | | |
| The table below summari | ses the geometric issu | ues observed across t | the polymeric chains and their |
| fit to the experimental da | ata. The red, orange | e, yellow and green s | segments indicate the fraction |
| of residues that contain c | outliers for $>=3, 2, 1$ | and 0 types of geom | netric quality criteria. A cyan |
| | | | 1 1 0 1 1 |

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 | А | 84 | 40% | 31% | • 27% | |



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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 mod | | | | | | | | |
| 1 | A:302-A:362 (61) | 0.33 | 7 | | | | | |

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 4 clusters and 1 single-model cluster was found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1221 atoms, of which 605 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called COP9 complex subunit 4.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|---|
| 1 | ٨ | 0.4 | Total | С | Н | Ν | 0 | S | 0 |
| 1 | А | 84 | 1221 | 380 | 605 | 106 | 128 | 2 | 0 |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| А | 289 | GLY | - | cloning artifact | UNP 088544 |
| А | 290 | SER | - | cloning artifact | UNP 088544 |
| А | 291 | SER | - | cloning artifact | UNP 088544 |
| А | 292 | GLY | - | cloning artifact | UNP 088544 |
| А | 293 | SER | - | cloning artifact | UNP 088544 |
| А | 294 | SER | - | cloning artifact | UNP 088544 |
| А | 295 | GLY | - | cloning artifact | UNP 088544 |
| А | 367 | SER | - | cloning artifact | UNP 088544 |
| А | 368 | GLY | - | cloning artifact | UNP 088544 |
| А | 369 | PRO | - | cloning artifact | UNP 088544 |
| А | 370 | SER | - | cloning artifact | UNP 088544 |
| А | 371 | SER | - | cloning artifact | UNP 088544 |
| А | 372 | GLY | - | cloning artifact | UNP 088544 |



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: COP9 complex subunit 4



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: COP9 complex subunit 4



4.2.2 Score per residue for model 2

• Molecule 1: COP9 complex subunit 4

Chain A: 48% 24% · 27%

4.2.3 Score per residue for model 3

• Molecule 1: COP9 complex subunit 4



4.2.4 Score per residue for model 4

• Molecule 1: COP9 complex subunit 4

| Chain A: | 38% | | 32% | • | 27% | - |
|--|------------------------------|------------------------------|--|--|--|--|
| 6289 8291 8294 6295 8294 6295 6295 6295 6295 8297 8298 8299 1299 | 1305 N308 L310 S313 | N318 1319 1320 F321 | L324 G325 L327 L328 L328 L328 E329 F331 A332 A333 K333 | A335 E336 K337 I338 A339 S340 S340 | E345 C346 R347 M348 N349 1352 D353 | G357 1358 1358 1359 1360 F361 E362 |
| T363 R364 A366 A366 A366 A366 A365 S371 S371 C372 G372 | | | | | | |

4.2.5 Score per residue for model 5

• Molecule 1: COP9 complex subunit 4



4.2.6 Score per residue for model 6

 \bullet Molecule 1: COP9 complex subunit 4

Chain A: 36% 33% · 27%

Tates Ta

4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: COP9 complex subunit 4



4.2.8 Score per residue for model 8

• Molecule 1: COP9 complex subunit 4



4.2.9 Score per residue for model 9

• Molecule 1: COP9 complex subunit 4



4.2.10 Score per residue for model 10

• Molecule 1: COP9 complex subunit 4





T363 R364 E365 A366 A366 C368 P369 P369 P369 S370 S371 C372 G372

4.2.11 Score per residue for model 11

• Molecule 1: COP9 complex subunit 4



4.2.12 Score per residue for model 12

• Molecule 1: COP9 complex subunit 4



4.2.13 Score per residue for model 13

• Molecule 1: COP9 complex subunit 4



4.2.14 Score per residue for model 14

 \bullet Molecule 1: COP9 complex subunit 4





P369 S370 S371 G372

4.2.15 Score per residue for model 15

• Molecule 1: COP9 complex subunit 4



4.2.16 Score per residue for model 16

• Molecule 1: COP9 complex subunit 4



4.2.17 Score per residue for model 17

• Molecule 1: COP9 complex subunit 4



4.2.18 Score per residue for model 18

 \bullet Molecule 1: COP9 complex subunit 4

Chain A: 30% 36% 7% 27%

4.2.19 Score per residue for model 19

• Molecule 1: COP9 complex subunit 4



4.2.20 Score per residue for model 20

• Molecule 1: COP9 complex subunit 4





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: torsion angle dynamics.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: target function.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CYANA | structure solution | 1.0.7 |
| CYANA | refinement | 1.0.7 |

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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 | А | 475 | 478 | 478 | 22 ± 5 |
| All | All | 9500 | 9560 | 9560 | 447 |

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 23.

| Atom 1 | Atom 2 | $Clach(\lambda)$ | Distance(Å) | Models | | |
|------------------|------------------|------------------|-------------|--------|-------|--|
| Atom-1 | Atom-2 | Clash(A) | Distance(A) | Worst | Total | |
| 1:A:324:LEU:CD2 | 1:A:328:LEU:HD11 | 0.91 | 1.96 | 17 | 7 | |
| 1:A:319:ILE:O | 1:A:359:VAL:HG22 | 0.89 | 1.66 | 5 | 6 | |
| 1:A:328:LEU:O | 1:A:330:ILE:HG23 | 0.80 | 1.77 | 6 | 16 | |
| 1:A:324:LEU:HD23 | 1:A:328:LEU:HD11 | 0.79 | 1.54 | 17 | 8 | |
| 1:A:321:PHE:CB | 1:A:332:ALA:HB1 | 0.79 | 2.07 | 3 | 19 | |
| 1:A:310:LEU:HD21 | 1:A:347:ARG:O | 0.78 | 1.77 | 13 | 6 | |
| 1:A:311:SER:O | 1:A:315:LEU:HD12 | 0.78 | 1.77 | 19 | 9 | |
| 1:A:320:THR:HG22 | 1:A:358:ILE:CD1 | 0.75 | 2.12 | 12 | 1 | |
| 1:A:320:THR:HG22 | 1:A:358:ILE:HD12 | 0.75 | 1.58 | 12 | 1 | |
| 1:A:324:LEU:HD12 | 1:A:359:VAL:HG21 | 0.74 | 1.58 | 16 | 2 | |
| 1:A:309:LEU:HD21 | 1:A:324:LEU:HD21 | 0.74 | 1.59 | 5 | 4 | |
| 1:A:351:PHE:CE2 | 1:A:360:HIS:CG | 0.73 | 2.76 | 5 | 1 | |
| 1:A:351:PHE:CZ | 1:A:360:HIS:CD2 | 0.72 | 2.77 | 5 | 1 | |
| 1:A:309:LEU:CD2 | 1:A:324:LEU:HD21 | 0.71 | 2.16 | 14 | 4 | |

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



| | | | | Models | | |
|------------------|--------------------------------|------|-------------|--------|-------|--|
| Atom-1 | tom-1 Atom-2 Clash(A) Distance | | Distance(A) | Worst | Total | |
| 1:A:321:PHE:HB2 | 1:A:332:ALA:HB1 | 0.71 | 1.62 | 3 | 10 | |
| 1:A:324:LEU:HD22 | 1:A:359:VAL:HG21 | 0.69 | 1.65 | 6 | 3 | |
| 1:A:308:ASN:OD1 | 1:A:327:LEU:HD11 | 0.68 | 1.88 | 18 | 1 | |
| 1:A:321:PHE:HB3 | 1:A:332:ALA:HB1 | 0.65 | 1.68 | 9 | 18 | |
| 1:A:321:PHE:CE1 | 1:A:359:VAL:CG2 | 0.64 | 2.79 | 20 | 1 | |
| 1:A:319:ILE:HG22 | 1:A:361:PHE:CE2 | 0.62 | 2.29 | 18 | 2 | |
| 1:A:311:SER:C | 1:A:315:LEU:HD12 | 0.62 | 2.15 | 19 | 3 | |
| 1:A:324:LEU:HD13 | 1:A:328:LEU:HD11 | 0.62 | 1.70 | 20 | 1 | |
| 1:A:310:LEU:HD11 | 1:A:347:ARG:O | 0.61 | 1.94 | 12 | 2 | |
| 1:A:305:ILE:HA | 1:A:328:LEU:HD22 | 0.60 | 1.70 | 6 | 4 | |
| 1:A:324:LEU:CD1 | 1:A:359:VAL:HG21 | 0.60 | 2.27 | 13 | 2 | |
| 1:A:309:LEU:CD1 | 1:A:338:ILE:HG22 | 0.60 | 2.27 | 20 | 6 | |
| 1:A:305:ILE:HG23 | 1:A:328:LEU:HD13 | 0.59 | 1.72 | 3 | 7 | |
| 1:A:319:ILE:HG23 | 1:A:324:LEU:HD12 | 0.59 | 1.75 | 8 | 1 | |
| 1:A:352:ILE:HG12 | 1:A:359:VAL:HG12 | 0.59 | 1.74 | 16 | 6 | |
| 1:A:321:PHE:CE2 | 1:A:357:GLY:O | 0.58 | 2.57 | 13 | 8 | |
| 1:A:309:LEU:HD13 | 1:A:338:ILE:HG22 | 0.58 | 1.76 | 20 | 6 | |
| 1:A:310:LEU:HD21 | 1:A:342:MET:CE | 0.58 | 2.28 | 17 | 2 | |
| 1:A:319:ILE:HG22 | 1:A:361:PHE:CZ | 0.56 | 2.36 | 18 | 1 | |
| 1:A:320:THR:HG22 | 1:A:358:ILE:HG12 | 0.55 | 1.79 | 1 | 1 | |
| 1:A:335:ALA:O | 1:A:339:ALA:CB | 0.54 | 2.55 | 11 | 18 | |
| 1:A:324:LEU:CD1 | 1:A:328:LEU:HD11 | 0.54 | 2.33 | 20 | 1 | |
| 1:A:309:LEU:HD22 | 1:A:338:ILE:HG22 | 0.54 | 1.78 | 4 | 3 | |
| 1:A:306:GLU:O | 1:A:342:MET:HE1 | 0.53 | 2.04 | 12 | 1 | |
| 1:A:321:PHE:CE1 | 1:A:359:VAL:HG23 | 0.53 | 2.38 | 20 | 1 | |
| 1:A:334:LYS:O | 1:A:338:ILE:CG1 | 0.53 | 2.56 | 8 | 4 | |
| 1:A:324:LEU:O | 1:A:328:LEU:HD12 | 0.53 | 2.04 | 2 | 7 | |
| 1:A:305:ILE:O | 1:A:309:LEU:HD12 | 0.52 | 2.04 | 11 | 4 | |
| 1:A:310:LEU:CD2 | 1:A:342:MET:CE | 0.52 | 2.87 | 17 | 2 | |
| 1:A:324:LEU:HD23 | 1:A:328:LEU:CD1 | 0.52 | 2.35 | 3 | 5 | |
| 1:A:324:LEU:O | 1:A:328:LEU:CD1 | 0.52 | 2.58 | 2 | 7 | |
| 1:A:308:ASN:CB | 1:A:328:LEU:CD2 | 0.52 | 2.87 | 4 | 6 | |
| 1:A:305:ILE:HG21 | 1:A:338:ILE:HD13 | 0.52 | 1.82 | 17 | 4 | |
| 1:A:325:GLY:O | 1:A:330:ILE:N | 0.51 | 2.43 | 4 | 20 | |
| 1:A:305:ILE:N | 1:A:305:ILE:CD1 | 0.51 | 2.74 | 17 | 4 | |
| 1:A:324:LEU:CD2 | 1:A:328:LEU:CD1 | 0.51 | 2.83 | 16 | 4 | |
| 1:A:332:ALA:O | 1:A:336:GLU:CB | 0.50 | 2.60 | 5 | 5 | |
| 1:A:324:LEU:HD13 | 1:A:328:LEU:CD1 | 0.50 | 2.36 | 20 | 1 | |
| 1:A:308:ASN:HD22 | 1:A:328:LEU:HD23 | 0.50 | 1.67 | 4 | 1 | |
| 1:A:308:ASN:CB | 1:A:328:LEU:HD23 | 0.50 | 2.37 | 9 | 6 | |
| 1:A:305:ILE:HG21 | 1:A:338:ILE:CD1 | 0.49 | 2.38 | 6 | 4 | |

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| | A L | | \mathbf{D} | Models | | |
|------------------|-----------------------|------|--------------|--------|-------|--|
| Atom-1 | Atom-1 Atom-2 Clash(A | | Distance(A) | Worst | Total | |
| 1:A:325:GLY:CA | 1:A:330:ILE:O | 0.49 | 2.60 | 14 | 17 | |
| 1:A:305:ILE:HG22 | 1:A:309:LEU:HD12 | 0.49 | 1.84 | 19 | 1 | |
| 1:A:335:ALA:O | 1:A:339:ALA:HB2 | 0.49 | 2.07 | 11 | 14 | |
| 1:A:351:PHE:CE2 | 1:A:360:HIS:CD2 | 0.48 | 3.00 | 5 | 1 | |
| 1:A:305:ILE:HD12 | 1:A:305:ILE:N | 0.48 | 2.23 | 4 | 2 | |
| 1:A:313:SER:HA | 1:A:361:PHE:CD1 | 0.48 | 2.43 | 8 | 2 | |
| 1:A:309:LEU:HD22 | 1:A:342:MET:SD | 0.48 | 2.49 | 16 | 1 | |
| 1:A:305:ILE:HG21 | 1:A:330:ILE:HD13 | 0.47 | 1.86 | 20 | 1 | |
| 1:A:305:ILE:HG22 | 1:A:338:ILE:HG21 | 0.47 | 1.86 | 6 | 2 | |
| 1:A:304:VAL:HG12 | 1:A:308:ASN:ND2 | 0.47 | 2.24 | 14 | 1 | |
| 1:A:321:PHE:CB | 1:A:332:ALA:CB | 0.47 | 2.87 | 3 | 2 | |
| 1:A:321:PHE:CE2 | 1:A:357:GLY:CA | 0.47 | 2.97 | 16 | 2 | |
| 1:A:343:ILE:HD11 | 1:A:348:MET:HE3 | 0.46 | 1.86 | 10 | 2 | |
| 1:A:332:ALA:O | 1:A:336:GLU:N | 0.46 | 2.46 | 18 | 16 | |
| 1:A:339:ALA:HB3 | 1:A:352:ILE:HD11 | 0.46 | 1.87 | 4 | 2 | |
| 1:A:305:ILE:N | 1:A:305:ILE:HD12 | 0.46 | 2.25 | 11 | 2 | |
| 1:A:320:THR:HG23 | 1:A:323:GLU:H | 0.46 | 1.71 | 16 | 1 | |
| 1:A:302:ARG:HA | 1:A:305:ILE:HD12 | 0.46 | 1.87 | 6 | 3 | |
| 1:A:353:ASP:O | 1:A:357:GLY:N | 0.45 | 2.50 | 5 | 7 | |
| 1:A:313:SER:CB | 1:A:361:PHE:CD1 | 0.45 | 3.00 | 10 | 1 | |
| 1:A:313:SER:HA | 1:A:361:PHE:CG | 0.45 | 2.46 | 5 | 4 | |
| 1:A:310:LEU:CD2 | 1:A:342:MET:SD | 0.45 | 3.05 | 12 | 1 | |
| 1:A:313:SER:HA | 1:A:361:PHE:CD2 | 0.45 | 2.46 | 13 | 4 | |
| 1:A:306:GLU:OE2 | 1:A:347:ARG:NH1 | 0.45 | 2.50 | 7 | 1 | |
| 1:A:317:ASN:O | 1:A:318:ASN:ND2 | 0.45 | 2.50 | 14 | 2 | |
| 1:A:319:ILE:CG2 | 1:A:361:PHE:CZ | 0.44 | 3.00 | 18 | 1 | |
| 1:A:308:ASN:HB2 | 1:A:328:LEU:CD2 | 0.44 | 2.42 | 1 | 8 | |
| 1:A:353:ASP:O | 1:A:357:GLY:CA | 0.44 | 2.66 | 18 | 4 | |
| 1:A:306:GLU:OE1 | 1:A:347:ARG:CD | 0.43 | 2.67 | 16 | 1 | |
| 1:A:306:GLU:OE1 | 1:A:347:ARG:NH1 | 0.43 | 2.50 | 17 | 1 | |
| 1:A:345:GLU:OE2 | 1:A:347:ARG:NH2 | 0.43 | 2.51 | 4 | 1 | |
| 1:A:342:MET:HE2 | 1:A:347:ARG:HB3 | 0.43 | 1.90 | 18 | 1 | |
| 1:A:310:LEU:CD2 | 1:A:310:LEU:N | 0.43 | 2.82 | 17 | 1 | |
| 1:A:351:PHE:CD1 | 1:A:351:PHE:C | 0.43 | 2.92 | 17 | 1 | |
| 1:A:309:LEU:CD1 | 1:A:338:ILE:CG2 | 0.43 | 2.96 | 20 | 1 | |
| 1:A:321:PHE:HB3 | 1:A:332:ALA:CB | 0.43 | 2.44 | 5 | 5 | |
| 1:A:308:ASN:HB3 | 1:A:328:LEU:CD2 | 0.43 | 2.44 | 16 | 6 | |
| 1:A:316:TYR:CD1 | 1:A:316:TYR:N | 0.43 | 2.87 | 9 | 1 | |
| 1:A:308:ASN:O | 1:A:312:ALA:CB | 0.43 | 2.67 | 9 | 2 | |
| 1:A:339:ALA:CB | 1:A:352:ILE:HD11 | 0.42 | 2.44 | 6 | 2 | |
| 1:A:306:GLU:OE2 | 1:A:347:ARG:CD | 0.42 | 2.68 | 18 | 1 | |

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| TOTM | 1UFM |
|------|------|
|------|------|

| | A + 2 | $C = h(\hat{\lambda})$ | \mathbf{D} : \mathbf{D} : \mathbf{D} | Moo | dels |
|------------------|------------------|------------------------|--|-------|-------|
| Atom-1 | Atom-2 | Clash(A) | Distance(A) | Worst | Total |
| 1:A:319:ILE:HD11 | 1:A:324:LEU:N | 0.42 | 2.29 | 3 | 1 |
| 1:A:304:VAL:HG12 | 1:A:308:ASN:HD22 | 0.42 | 1.73 | 14 | 1 |
| 1:A:327:LEU:HD12 | 1:A:327:LEU:O | 0.42 | 2.14 | 6 | 1 |
| 1:A:308:ASN:HB3 | 1:A:328:LEU:HD23 | 0.41 | 1.92 | 1 | 1 |
| 1:A:342:MET:HE2 | 1:A:347:ARG:CB | 0.41 | 2.44 | 18 | 1 |
| 1:A:319:ILE:HG21 | 1:A:324:LEU:HD13 | 0.41 | 1.90 | 1 | 3 |
| 1:A:306:GLU:O | 1:A:342:MET:CE | 0.41 | 2.68 | 10 | 1 |
| 1:A:330:ILE:CD1 | 1:A:338:ILE:HD12 | 0.41 | 2.44 | 6 | 1 |
| 1:A:338:ILE:O | 1:A:342:MET:CG | 0.41 | 2.68 | 13 | 1 |
| 1:A:313:SER:HB2 | 1:A:361:PHE:CD1 | 0.41 | 2.50 | 10 | 1 |
| 1:A:324:LEU:HD22 | 1:A:335:ALA:HB1 | 0.41 | 1.92 | 16 | 1 |
| 1:A:325:GLY:C | 1:A:330:ILE:O | 0.41 | 2.59 | 2 | 9 |
| 1:A:362:GLU:OE1 | 1:A:362:GLU:CA | 0.41 | 2.69 | 10 | 1 |
| 1:A:325:GLY:O | 1:A:329:GLU:N | 0.41 | 2.53 | 13 | 2 |
| 1:A:306:GLU:O | 1:A:342:MET:HE3 | 0.41 | 2.16 | 3 | 1 |
| 1:A:327:LEU:O | 1:A:327:LEU:HD12 | 0.41 | 2.16 | 4 | 1 |
| 1:A:353:ASP:N | 1:A:358:ILE:O | 0.41 | 2.54 | 5 | 1 |
| 1:A:324:LEU:HD11 | 1:A:361:PHE:HZ | 0.41 | 1.75 | 17 | 1 |
| 1:A:304:VAL:O | 1:A:308:ASN:CG | 0.41 | 2.60 | 17 | 2 |
| 1:A:304:VAL:CG1 | 1:A:308:ASN:ND2 | 0.41 | 2.84 | 14 | 1 |
| 1:A:330:ILE:HD12 | 1:A:334:LYS:HB3 | 0.41 | 1.92 | 18 | 1 |
| 1:A:304:VAL:O | 1:A:308:ASN:OD1 | 0.40 | 2.39 | 12 | 1 |
| 1:A:306:GLU:CG | 1:A:342:MET:SD | 0.40 | 3.09 | 10 | 1 |
| 1:A:343:ILE:HG13 | 1:A:348:MET:CE | 0.40 | 2.46 | 10 | 1 |
| 1:A:346:GLY:O | 1:A:347:ARG:C | 0.40 | 2.60 | 17 | 1 |
| 1:A:313:SER:O | 1:A:362:GLU:O | 0.40 | 2.40 | 20 | 1 |
| 1:A:305:ILE:CG2 | 1:A:338:ILE:HG21 | 0.40 | 2.46 | 6 | 1 |
| 1:A:325:GLY:O | 1:A:330:ILE:O | 0.40 | 2.40 | 17 | 1 |

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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 | А | 61/84~(73%) | 59 ± 1 (97 $\pm1\%$) | $2\pm1 (3\pm1\%)$ | 0±0 (0±0%) | 100 100 |



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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|---------|----------|-------------|
| All | All | 1220/1680~(73%) | 1189~(97%) | 31~(3%) | 0 (0%) | 100 100 |

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Pe | rce | entile | es |
|-----|-------|-----------------|-------------------------|---------------------|----|-----|--------|----|
| 1 | А | 50/66~(76%) | 40 ± 2 (81 $\pm4\%$) | $10\pm2~(19\pm4\%)$ | | 4 | 35 | |
| All | All | 1000/1320~(76%) | 806 (81%) | 194 (19%) | | 4 | 35 | |

All 24 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 | А | 318 | ASN | 20 |
| 1 | А | 328 | LEU | 20 |
| 1 | А | 340 | SER | 20 |
| 1 | А | 327 | LEU | 18 |
| 1 | А | 302 | ARG | 14 |
| 1 | А | 311 | SER | 14 |
| 1 | А | 349 | ASN | 12 |
| 1 | А | 334 | LYS | 11 |
| 1 | А | 360 | HIS | 11 |
| 1 | А | 341 | GLN | 9 |
| 1 | А | 314 | LYS | 8 |
| 1 | А | 309 | LEU | 8 |
| 1 | А | 317 | ASN | 6 |
| 1 | А | 356 | ASP | 5 |
| 1 | А | 337 | LYS | 4 |
| 1 | А | 310 | LEU | 3 |
| 1 | А | 304 | VAL | 3 |
| 1 | А | 308 | ASN | 2 |
| 1 | А | 306 | GLU | 1 |
| 1 | А | 342 | MET | 1 |
| 1 | А | 344 | THR | 1 |
| 1 | А | 324 | LEU | 1 |



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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | А | 348 | MET | 1 |
| 1 | А | 313 | SER | 1 |

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

