# WORLDWIDE PDB PROTEIN DATA BANK

# wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 08:13 pm BST

| | | |
|---|---|---|
| PDB ID | : | 6HXW |
| Title | : | structure of human CD73 in complex with antibody IPH53 |
| Authors | : | Roussel, A.; Amigues, B. |
| Deposited on | : | 2018-10-18 |
| Resolution | : | 2.78 Å(reported) |

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

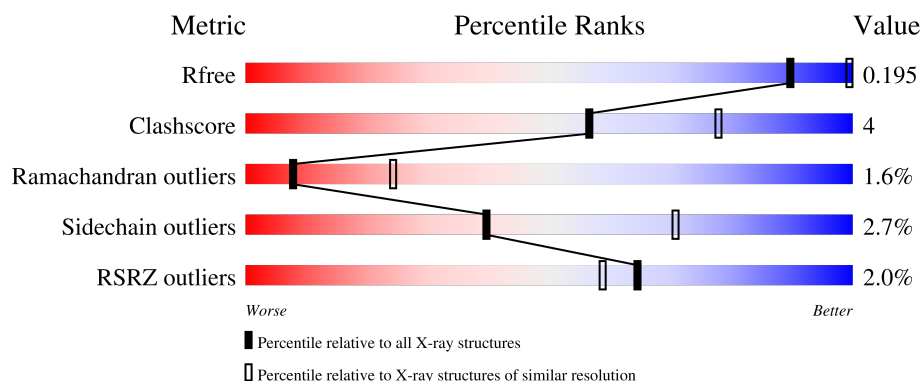| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 3.0 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4 | : | 9.0.003 (Gargrove) |
| Density-Fitness | : | 1.0.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 1   Overall quality at a glance  ⓘ

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 Å.

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

| Metric | Percentile Ranks | Value |
|--------|------------------|-------|
| Rfree | | 0.195 |
| Clashscore | | 4 |
| Ramachandran outliers | | 1.6% |
| Sidechain outliers | | 2.7% |
| RSRZ outliers | | 2.0% |

*Worse*                                       *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------|--------------------------|------------------------------------------------------|
| R$_{free}$ | 164625 | 4924 (2.80-2.76) |
| Clashscore | 180529 | 5458 (2.80-2.76) |
| Ramachandran outliers | 177936 | 5386 (2.80-2.76) |
| Sidechain outliers | 177891 | 5388 (2.80-2.76) |
| RSRZ outliers | 164620 | 4926 (2.80-2.76) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 527 | %<br>89%     9%  • |
| 1 | B | 527 | %<br>90%     9%  • |
| 2 | C | 231 | 2%<br>80%     13%     7% |
| 2 | H | 231 | 6%<br>81%     11%     7% |
| 3 | D | 209 | %<br>85%     13%  • |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | L | 209 | 3%     78%     18% |

# 2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 15507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 5'-nucleotidase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 1 | A | 523 | Total 4074 | C 2588 | N 700 | O 767 | S 19 | 0 | 0 | 0 |
| 1 | B | 523 | Total 4071 | C 2587 | N 700 | O 765 | S 19 | 0 | 0 | 0 |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 548 | HIS | PHE | conflict | UNP P21589 |
| A | 549 | HIS | SER | conflict | UNP P21589 |
| A | 550 | HIS | THR | conflict | UNP P21589 |
| A | 551 | HIS | GLY | conflict | UNP P21589 |
| A | 552 | HIS | SER | conflict | UNP P21589 |
| B | 548 | HIS | PHE | conflict | UNP P21589 |
| B | 549 | HIS | SER | conflict | UNP P21589 |
| B | 550 | HIS | THR | conflict | UNP P21589 |
| B | 551 | HIS | GLY | conflict | UNP P21589 |
| B | 552 | HIS | SER | conflict | UNP P21589 |

- Molecule 2 is a protein called IPH53 heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 2 | C | 215 | Total 1642 | C 1044 | N 276 | O 316 | S 6 | 698 | 0 | 0 |
| 2 | H | 215 | Total 1642 | C 1044 | N 276 | O 316 | S 6 | 0 | 0 | 0 |

- Molecule 3 is a protein called IPH53 light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 3 | D | 209 | Total 1618 | C 1015 | N 269 | O 329 | S 5 | 816 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | L | 209 | 1618 | 1015 | 269 | 329 | 5 | 0 | 0 | 0 |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



NAG

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| | | | Total | C | N | O | | |
| 4 | A | 1 | 14 | 8 | 1 | 5 | 0 | 0 |
| 4 | B | 1 | 14 | 8 | 1 | 5 | 0 | 0 |

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| | | | Total | Zn | | |
| 5 | A | 2 | 2 | 2 | 0 | 0 |
| 5 | B | 2 | 2 | 2 | 0 | 0 |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| | | | Total | O | | |
| 6 | A | 229 | 229 | 229 | 0 | 0 |

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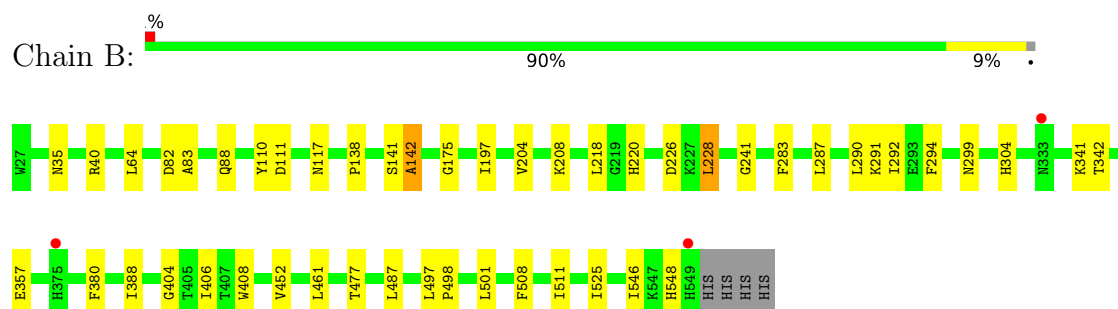| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6 | B | 273 | Total 273 | O 273 | 0 | 0 |
| 6 | C | 62 | Total 62 | O 62 | 0 | 0 |
| 6 | D | 66 | Total 66 | O 66 | 0 | 0 |
| 6 | H | 93 | Total 93 | O 93 | 0 | 0 |
| 6 | L | 87 | Total 87 | O 87 | 0 | 0 |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
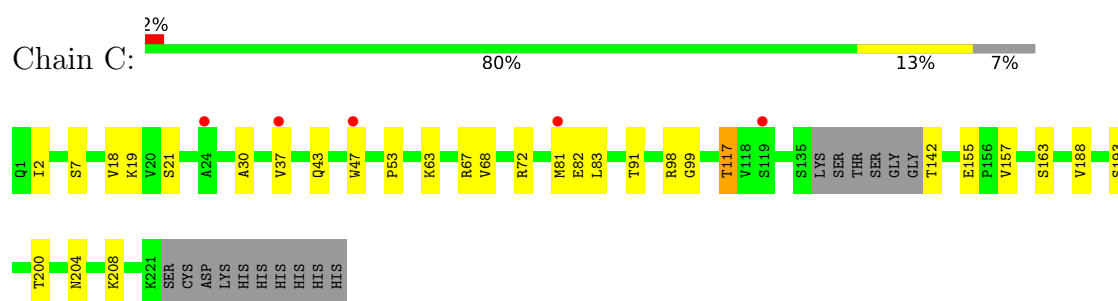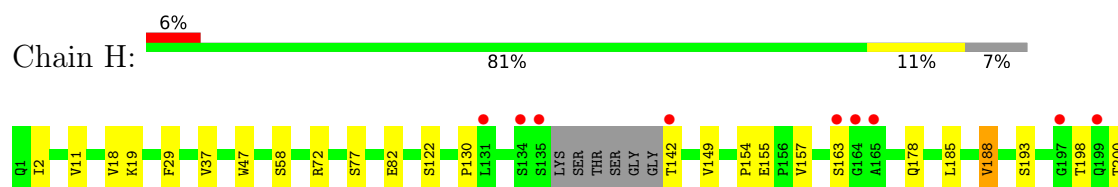
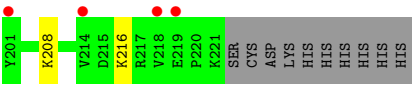- Molecule 1: 5'-nucleotidase

Chain A:

- Molecule 1: 5'-nucleotidase

Chain B:

- Molecule 2: IPH53 heavy chain

Chain C:

- Molecule 2: IPH53 heavy chain

Chain H:

Y201 K208 V214 D215 K216 R217 V218 E219 P220 K221 SER CYS ASP LYS HIS HIS HIS HIS HIS HIS

• Molecule 3: IPH53 light chain

Chain D:

85%    13%

I2 S7 L11 S12 V15 K24 V33 Q37 P40 L47 V58 F62 G68 T69 D70 L78 I83 Q89 L95 L103 E104 I105 I116 K125 V131 N137 E142 D150 S158 Q165 D166 S167 S173 T205

R210

• Molecule 3: IPH53 light chain

Chain L:

3%

78%    18%

I2 S7 P8 S9 K24 Q27 T30 N31 D32 V33 P40 R54 Y55 T56 G57 V58 G68 T69 L78 I83 Q89 S93 S94 L95 T96 F97 L103 E104 I105 I116 F117 P118 L124 K125 S126 G127 T128 V131 L134 L135 N136 N137 K148

V149 D150 N151 A152 S158 S167 S170 S173 L174 T177 L178 K182 Y191 A192 C193 T205 K206 S207 F208 N209 R210

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 195.35Å   209.43Å   65.06Å<br>90.00°     90.00°     90.00° | Depositor |
| Resolution (Å) | 48.84  –  2.78<br>48.84  –  2.78 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.3 (48.84-2.78)<br>99.5 (48.84-2.78) | Depositor<br>EDS |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $<I/\sigma(I)>$ [1] | 1.90 (at 2.77Å) | Xtriage |
| Refinement program | BUSTER 2.10.3 | Depositor |
| R, $R_{free}$ | 0.192  ,  0.232<br>0.193  ,  0.195 | Depositor<br>DCC |
| $R_{free}$ test set | 3773 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 52.3 | Xtriage |
| Anisotropy | 0.885 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 66.4 | EDS |
| L-test for twinning [2] | $<|L|> = 0.49, <L^2> = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o,F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 15507 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 79.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|------|---------|------|---------|
| | | RMSZ | #$|Z|$ >5 | RMSZ | #$|Z|$ >5 |
| 1 | A | 0.50 | 0/4161 | 0.73 | 0/5639 |
| 1 | B | 0.52 | 0/4158 | 0.72 | 0/5635 |
| 2 | C | 0.44 | 0/1685 | 0.72 | 0/2295 |
| 2 | H | 0.47 | 0/1685 | 0.70 | 0/2295 |
| 3 | D | 0.43 | 0/1653 | 0.75 | 1/2245 (0.0%) |
| 3 | L | 0.46 | 0/1653 | 0.78 | 1/2245 (0.0%) |
| All | All | 0.48 | 0/14995 | 0.73 | 2/20354 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|-----|-----------|---------|
| 3 | L | 7 | SER | N-CA-C | -5.45 | 96.28 | 111.00 |
| 3 | D | 7 | SER | N-CA-C | -5.13 | 97.16 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4074 | 0 | 4037 | 32 | 0 |
| 1 | B | 4071 | 0 | 4029 | 31 | 0 |
| 2 | C | 1642 | 0 | 1601 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | H | 1642 | 0 | 1601 | 10 | 0 |
| 3 | D | 1618 | 0 | 1570 | 13 | 0 |
| 3 | L | 1618 | 0 | 1570 | 23 | 0 |
| 4 | A | 14 | 0 | 13 | 0 | 0 |
| 4 | B | 14 | 0 | 13 | 0 | 0 |
| 5 | A | 2 | 0 | 0 | 0 | 0 |
| 5 | B | 2 | 0 | 0 | 0 | 0 |
| 6 | A | 229 | 0 | 0 | 1 | 0 |
| 6 | B | 273 | 0 | 0 | 0 | 0 |
| 6 | C | 62 | 0 | 0 | 1 | 0 |
| 6 | D | 66 | 0 | 0 | 0 | 0 |
| 6 | H | 93 | 0 | 0 | 0 | 0 |
| 6 | L | 87 | 0 | 0 | 0 | 0 |
| All | All | 15507 | 0 | 14434 | 117 | 0 |

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 4.

The worst 5 of 117 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 3:D:89:GLN:HE21 | 3:D:95:LEU:HD11 | 1.22 | 1.03 |
| 3:D:24:LYS:HE2 | 3:D:70:ASP:OD1 | 1.62 | 0.99 |
| 3:L:116:ILE:HD11 | 3:L:193:CYS:HB3 | 1.49 | 0.93 |
| 1:A:388:ILE:HG13 | 1:A:497:LEU:HD13 | 1.53 | 0.90 |
| 3:L:30:THR:HG22 | 3:L:31:ASN:H | 1.35 | 0.90 |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|-------------|-----|
| 1 | A | 521/527 (99%) | 489 (94%) | 29 (6%) | 3 (1%) | 22 | 48 |
| 1 | B | 521/527 (99%) | 484 (93%) | 35 (7%) | 2 (0%) | 30 | 58 |
| 2 | C | 211/231 (91%) | 194 (92%) | 14 (7%) | 3 (1%) | 9 | 27 |
| 2 | H | 211/231 (91%) | 195 (92%) | 12 (6%) | 4 (2%) | 6 | 20 |
| 3 | D | 207/209 (99%) | 180 (87%) | 16 (8%) | 11 (5%) | 1 | 4 |
| 3 | L | 207/209 (99%) | 182 (88%) | 18 (9%) | 7 (3%) | 3 | 9 |
| All | All | 1878/1934 (97%) | 1724 (92%) | 124 (7%) | 30 (2%) | 8 | 24 |

5 of 30 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 163 | SER |
| 3 | D | 40 | PRO |
| 3 | D | 150 | ASP |
| 3 | D | 165 | GLN |
| 3 | D | 167 | SER |

### 5.3.2   Protein sidechains   ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|-------------|-----|
| 1 | A | 448/455 (98%) | 444 (99%) | 4 (1%) | 75 | 91 |
| 1 | B | 446/455 (98%) | 444 (100%) | 2 (0%) | 89 | 96 |
| 2 | C | 180/195 (92%) | 168 (93%) | 12 (7%) | 13 | 35 |
| 2 | H | 180/195 (92%) | 171 (95%) | 9 (5%) | 20 | 48 |
| 3 | D | 185/185 (100%) | 178 (96%) | 7 (4%) | 28 | 59 |
| 3 | L | 185/185 (100%) | 175 (95%) | 10 (5%) | 18 | 45 |
| All | All | 1624/1670 (97%) | 1580 (97%) | 44 (3%) | 40 | 71 |

5 of 44 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | H | 142 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | L | 93 | SER |
| 2 | H | 155 | GLU |
| 2 | H | 200 | THR |
| 3 | L | 116 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 69 | GLN |
| 1 | B | 304 | HIS |
| 1 | B | 549 | HIS |
| 3 | D | 53 | ASN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | #$\|Z\| > 2$ | Counts | RMSZ | #$\|Z\| > 2$ |
| 4 | NAG | B | 601 | 1 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.77 | 2 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|---------|--------|------|---------|
| | | | | | Counts | RMSZ | $\#|Z| > 2$ | Counts | RMSZ | $\#|Z| > 2$ |
| 4 | NAG | A | 601 | 1 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.73 | 1 (5%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 4 | NAG | B | 601 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 601 | 1 | - | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|------|-----------|---------|
| 4 | B | 601 | NAG | C1-O5-C5 | 2.12 | 115.06 | 112.19 |
| 4 | B | 601 | NAG | O5-C1-C2 | -2.11 | 107.96 | 111.29 |
| 4 | A | 601 | NAG | O5-C1-C2 | -2.09 | 107.99 | 111.29 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7   Other polymers  ⓘ

There are no such residues in this entry.

## 5.8   Polymer linkage issues  ⓘ

There are no chain breaks in this entry.

# 6   Fit of model and data ⓘ

## 6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|-----|-------|----------|--------|---------|----|----|-------------|-------|
| 1 | A | 523/527 (99%) | -0.32 | 3 (0%) | 85 | 82 | 38, 54, 81, 120 | 0 |
| 1 | B | 523/527 (99%) | -0.35 | 3 (0%) | 85 | 82 | 37, 53, 75, 118 | 0 |
| 2 | C | 119/231 (51%) | 0.33 | 5 (4%) | 41 | 36 | 53, 88, 122, 145 | 0 |
| 2 | H | 215/231 (93%) | 0.07 | 13 (6%) | 29 | 24 | 42, 62, 110, 145 | 0 |
| 3 | D | 104/209 (49%) | 0.39 | 3 (2%) | 54 | 48 | 53, 85, 122, 161 | 0 |
| 3 | L | 209/209 (100%) | 0.18 | 7 (3%) | 49 | 44 | 41, 71, 119, 136 | 0 |
| All | All | 1693/1934 (87%) | -0.13 | 34 (2%) | 64 | 59 | 37, 57, 109, 161 | 0 |

The worst 5 of 34 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | D | 105 | ILE | 6.4 |
| 2 | H | 164 | GLY | 4.6 |
| 2 | H | 165 | ALA | 4.0 |
| 1 | B | 549 | HIS | 3.9 |
| 1 | A | 334 | TYR | 3.6 |

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

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

## 6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors($\text{Å}^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------------------------|-------|
| 4 | NAG | A | 601 | 14/15 | 0.86 | 0.12 | 90,96,99,99 | 0 |
| 4 | NAG | B | 601 | 14/15 | 0.88 | 0.10 | 72,77,81,82 | 0 |
| 5 | ZN | A | 603 | 1/1 | 0.96 | 0.11 | 74,74,74,74 | 0 |
| 5 | ZN | A | 602 | 1/1 | 0.97 | 0.10 | 56,56,56,56 | 0 |
| 5 | ZN | B | 602 | 1/1 | 0.98 | 0.10 | 51,51,51,51 | 0 |
| 5 | ZN | B | 603 | 1/1 | 0.98 | 0.09 | 58,58,58,58 | 0 |

## 6.5   Other polymers ⓘ

There are no such residues in this entry.