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

Feb 21, 2024 – 04:09 PM EST

| | | |
|---|---|---|
| PDB ID | : | 4NSC |
| Title | : | Crystal Structure of CBARA1 in the Apo-form |
| Authors | : | Wang, L.; Yang, X.; Li, S.; Shen, Y. |
| Deposited on | : | 2013-11-28 |
| Resolution | : | 3.20 Å(reported) |

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp
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:

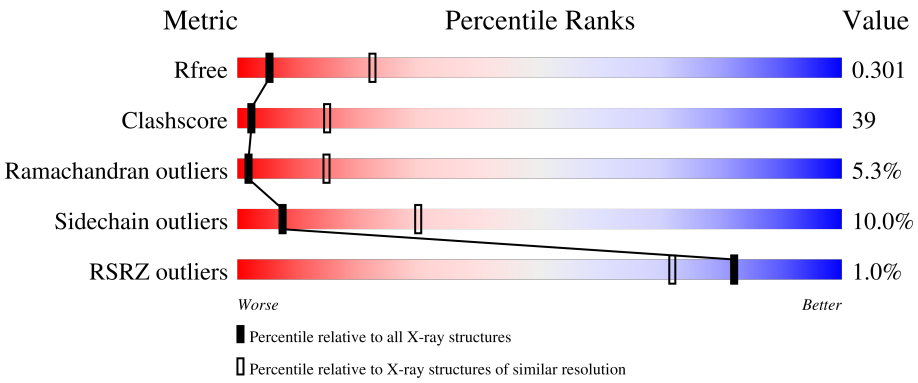
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & 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:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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 | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1133 (3.20-3.20) |
| Clashscore | 141614 | 1253 (3.20-3.20) |
| Ramachandran outliers | 138981 | 1234 (3.20-3.20) |
| Sidechain outliers | 138945 | 1233 (3.20-3.20) |
| RSRZ outliers | 127900 | 1095 (3.20-3.20) |

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 | 401 | 2% 29% 39% 8% 23% |
| 1 | B | 401 | 35% 36% 7% • 21% |
| 1 | C | 401 | % 28% 47% 6% • 18% |
| 1 | D | 401 | % 37% 36% 7% • 19% |
| 1 | E | 401 | 35% 40% 6% • 18% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 401 | 34% 35% 7% • 23% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15349 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 Calcium uptake protein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 310 | 2472 | 1583 | 419 | 454 | 16 | 0 | 0 | 0 |
| 1 | B | 316 | 2539 | 1622 | 426 | 473 | 18 | 0 | 0 | 0 |
| 1 | C | 330 | 2619 | 1673 | 442 | 486 | 18 | 0 | 0 | 0 |
| 1 | D | 326 | 2604 | 1662 | 438 | 487 | 17 | 0 | 0 | 0 |
| 1 | E | 330 | 2598 | 1657 | 439 | 487 | 15 | 0 | 0 | 0 |
| 1 | F | 310 | 2504 | 1601 | 422 | 468 | 13 | 0 | 0 | 0 |

There are 126 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 76 | MET | - | expression tag | UNP Q9BPX6 |
| A | 77 | HIS | - | expression tag | UNP Q9BPX6 |
| A | 78 | HIS | - | expression tag | UNP Q9BPX6 |
| A | 79 | HIS | - | expression tag | UNP Q9BPX6 |
| A | 80 | HIS | - | expression tag | UNP Q9BPX6 |
| A | 81 | HIS | - | expression tag | UNP Q9BPX6 |
| A | 82 | HIS | - | expression tag | UNP Q9BPX6 |
| A | 83 | SER | - | expression tag | UNP Q9BPX6 |
| A | 84 | SER | - | expression tag | UNP Q9BPX6 |
| A | 85 | GLY | - | expression tag | UNP Q9BPX6 |
| A | 86 | LEU | - | expression tag | UNP Q9BPX6 |
| A | 87 | GLU | - | expression tag | UNP Q9BPX6 |
| A | 88 | VAL | - | expression tag | UNP Q9BPX6 |
| A | 89 | LEU | - | expression tag | UNP Q9BPX6 |
| A | 90 | PHE | - | expression tag | UNP Q9BPX6 |
| A | 91 | GLN | - | expression tag | UNP Q9BPX6 |
| A | 92 | GLY | - | expression tag | UNP Q9BPX6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 93 | PRO | - | expression tag | UNP Q9BPX6 |
| A | 94 | GLY | - | expression tag | UNP Q9BPX6 |
| A | 95 | SER | - | expression tag | UNP Q9BPX6 |
| A | 96 | MET | - | expression tag | UNP Q9BPX6 |
| B | 76 | MET | - | expression tag | UNP Q9BPX6 |
| B | 77 | HIS | - | expression tag | UNP Q9BPX6 |
| B | 78 | HIS | - | expression tag | UNP Q9BPX6 |
| B | 79 | HIS | - | expression tag | UNP Q9BPX6 |
| B | 80 | HIS | - | expression tag | UNP Q9BPX6 |
| B | 81 | HIS | - | expression tag | UNP Q9BPX6 |
| B | 82 | HIS | - | expression tag | UNP Q9BPX6 |
| B | 83 | SER | - | expression tag | UNP Q9BPX6 |
| B | 84 | SER | - | expression tag | UNP Q9BPX6 |
| B | 85 | GLY | - | expression tag | UNP Q9BPX6 |
| B | 86 | LEU | - | expression tag | UNP Q9BPX6 |
| B | 87 | GLU | - | expression tag | UNP Q9BPX6 |
| B | 88 | VAL | - | expression tag | UNP Q9BPX6 |
| B | 89 | LEU | - | expression tag | UNP Q9BPX6 |
| B | 90 | PHE | - | expression tag | UNP Q9BPX6 |
| B | 91 | GLN | - | expression tag | UNP Q9BPX6 |
| B | 92 | GLY | - | expression tag | UNP Q9BPX6 |
| B | 93 | PRO | - | expression tag | UNP Q9BPX6 |
| B | 94 | GLY | - | expression tag | UNP Q9BPX6 |
| B | 95 | SER | - | expression tag | UNP Q9BPX6 |
| B | 96 | MET | - | expression tag | UNP Q9BPX6 |
| C | 76 | MET | - | expression tag | UNP Q9BPX6 |
| C | 77 | HIS | - | expression tag | UNP Q9BPX6 |
| C | 78 | HIS | - | expression tag | UNP Q9BPX6 |
| C | 79 | HIS | - | expression tag | UNP Q9BPX6 |
| C | 80 | HIS | - | expression tag | UNP Q9BPX6 |
| C | 81 | HIS | - | expression tag | UNP Q9BPX6 |
| C | 82 | HIS | - | expression tag | UNP Q9BPX6 |
| C | 83 | SER | - | expression tag | UNP Q9BPX6 |
| C | 84 | SER | - | expression tag | UNP Q9BPX6 |
| C | 85 | GLY | - | expression tag | UNP Q9BPX6 |
| C | 86 | LEU | - | expression tag | UNP Q9BPX6 |
| C | 87 | GLU | - | expression tag | UNP Q9BPX6 |
| C | 88 | VAL | - | expression tag | UNP Q9BPX6 |
| C | 89 | LEU | - | expression tag | UNP Q9BPX6 |
| C | 90 | PHE | - | expression tag | UNP Q9BPX6 |
| C | 91 | GLN | - | expression tag | UNP Q9BPX6 |
| C | 92 | GLY | - | expression tag | UNP Q9BPX6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 93 | PRO | - | expression tag | UNP Q9BPX6 |
| C | 94 | GLY | - | expression tag | UNP Q9BPX6 |
| C | 95 | SER | - | expression tag | UNP Q9BPX6 |
| C | 96 | MET | - | expression tag | UNP Q9BPX6 |
| D | 76 | MET | - | expression tag | UNP Q9BPX6 |
| D | 77 | HIS | - | expression tag | UNP Q9BPX6 |
| D | 78 | HIS | - | expression tag | UNP Q9BPX6 |
| D | 79 | HIS | - | expression tag | UNP Q9BPX6 |
| D | 80 | HIS | - | expression tag | UNP Q9BPX6 |
| D | 81 | HIS | - | expression tag | UNP Q9BPX6 |
| D | 82 | HIS | - | expression tag | UNP Q9BPX6 |
| D | 83 | SER | - | expression tag | UNP Q9BPX6 |
| D | 84 | SER | - | expression tag | UNP Q9BPX6 |
| D | 85 | GLY | - | expression tag | UNP Q9BPX6 |
| D | 86 | LEU | - | expression tag | UNP Q9BPX6 |
| D | 87 | GLU | - | expression tag | UNP Q9BPX6 |
| D | 88 | VAL | - | expression tag | UNP Q9BPX6 |
| D | 89 | LEU | - | expression tag | UNP Q9BPX6 |
| D | 90 | PHE | - | expression tag | UNP Q9BPX6 |
| D | 91 | GLN | - | expression tag | UNP Q9BPX6 |
| D | 92 | GLY | - | expression tag | UNP Q9BPX6 |
| D | 93 | PRO | - | expression tag | UNP Q9BPX6 |
| D | 94 | GLY | - | expression tag | UNP Q9BPX6 |
| D | 95 | SER | - | expression tag | UNP Q9BPX6 |
| D | 96 | MET | - | expression tag | UNP Q9BPX6 |
| E | 76 | MET | - | expression tag | UNP Q9BPX6 |
| E | 77 | HIS | - | expression tag | UNP Q9BPX6 |
| E | 78 | HIS | - | expression tag | UNP Q9BPX6 |
| E | 79 | HIS | - | expression tag | UNP Q9BPX6 |
| E | 80 | HIS | - | expression tag | UNP Q9BPX6 |
| E | 81 | HIS | - | expression tag | UNP Q9BPX6 |
| E | 82 | HIS | - | expression tag | UNP Q9BPX6 |
| E | 83 | SER | - | expression tag | UNP Q9BPX6 |
| E | 84 | SER | - | expression tag | UNP Q9BPX6 |
| E | 85 | GLY | - | expression tag | UNP Q9BPX6 |
| E | 86 | LEU | - | expression tag | UNP Q9BPX6 |
| E | 87 | GLU | - | expression tag | UNP Q9BPX6 |
| E | 88 | VAL | - | expression tag | UNP Q9BPX6 |
| E | 89 | LEU | - | expression tag | UNP Q9BPX6 |
| E | 90 | PHE | - | expression tag | UNP Q9BPX6 |
| E | 91 | GLN | - | expression tag | UNP Q9BPX6 |
| E | 92 | GLY | - | expression tag | UNP Q9BPX6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 93 | PRO | - | expression tag | UNP Q9BPX6 |
| E | 94 | GLY | - | expression tag | UNP Q9BPX6 |
| E | 95 | SER | - | expression tag | UNP Q9BPX6 |
| E | 96 | MET | - | expression tag | UNP Q9BPX6 |
| F | 76 | MET | - | expression tag | UNP Q9BPX6 |
| F | 77 | HIS | - | expression tag | UNP Q9BPX6 |
| F | 78 | HIS | - | expression tag | UNP Q9BPX6 |
| F | 79 | HIS | - | expression tag | UNP Q9BPX6 |
| F | 80 | HIS | - | expression tag | UNP Q9BPX6 |
| F | 81 | HIS | - | expression tag | UNP Q9BPX6 |
| F | 82 | HIS | - | expression tag | UNP Q9BPX6 |
| F | 83 | SER | - | expression tag | UNP Q9BPX6 |
| F | 84 | SER | - | expression tag | UNP Q9BPX6 |
| F | 85 | GLY | - | expression tag | UNP Q9BPX6 |
| F | 86 | LEU | - | expression tag | UNP Q9BPX6 |
| F | 87 | GLU | - | expression tag | UNP Q9BPX6 |
| F | 88 | VAL | - | expression tag | UNP Q9BPX6 |
| F | 89 | LEU | - | expression tag | UNP Q9BPX6 |
| F | 90 | PHE | - | expression tag | UNP Q9BPX6 |
| F | 91 | GLN | - | expression tag | UNP Q9BPX6 |
| F | 92 | GLY | - | expression tag | UNP Q9BPX6 |
| F | 93 | PRO | - | expression tag | UNP Q9BPX6 |
| F | 94 | GLY | - | expression tag | UNP Q9BPX6 |
| F | 95 | SER | - | expression tag | UNP Q9BPX6 |
| F | 96 | MET | - | expression tag | UNP Q9BPX6 |

- Molecule 2 is water.

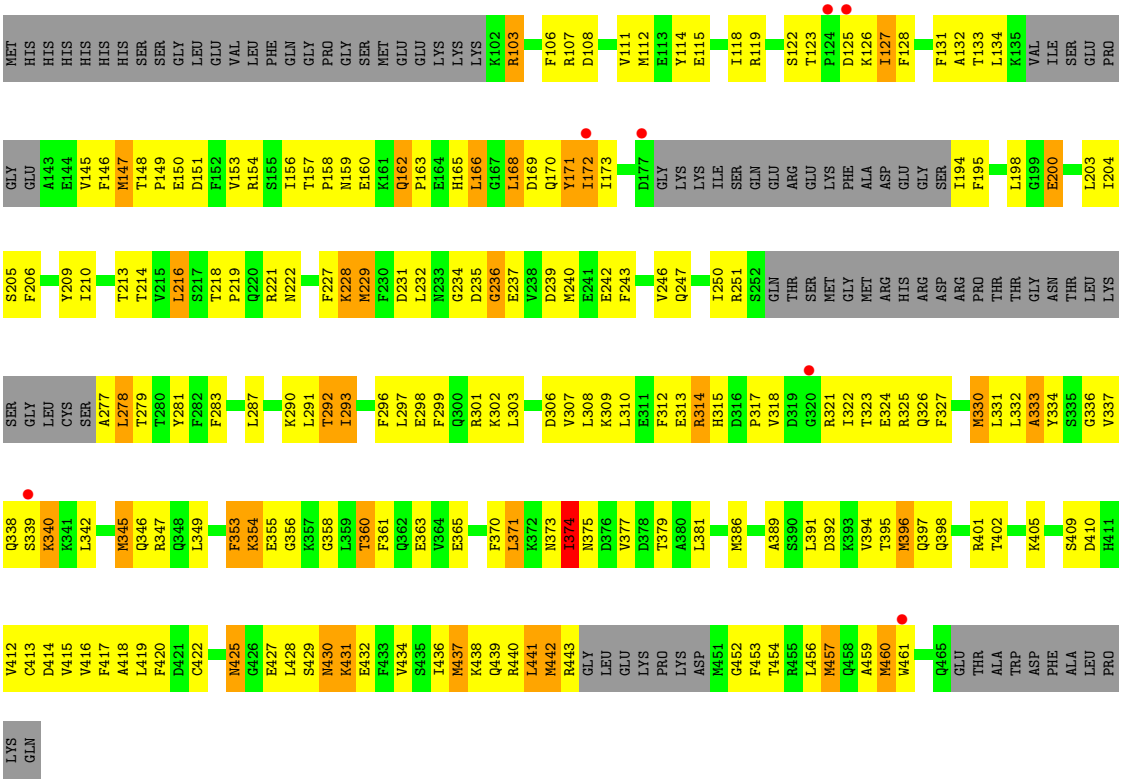
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 2 | A | 4 | 4 | 4 | 0 | 0 |
| | | | Total | O | | |
| 2 | B | 3 | 3 | 3 | 0 | 0 |
| | | | Total | O | | |
| 2 | C | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 2 | D | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 2 | F | 4 | 4 | 4 | 0 | 0 |

# 3 Residue-property plots (i)

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.

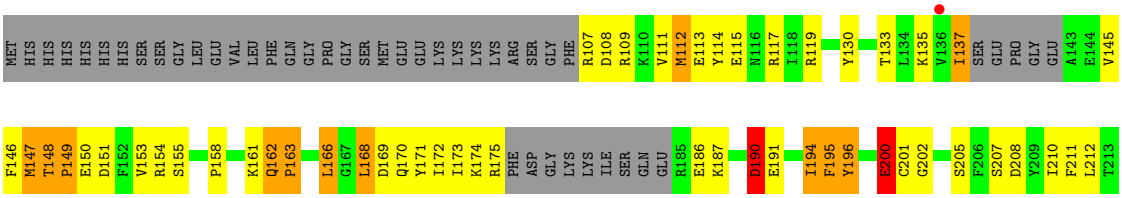
• Molecule 1: Calcium uptake protein 1, mitochondrial

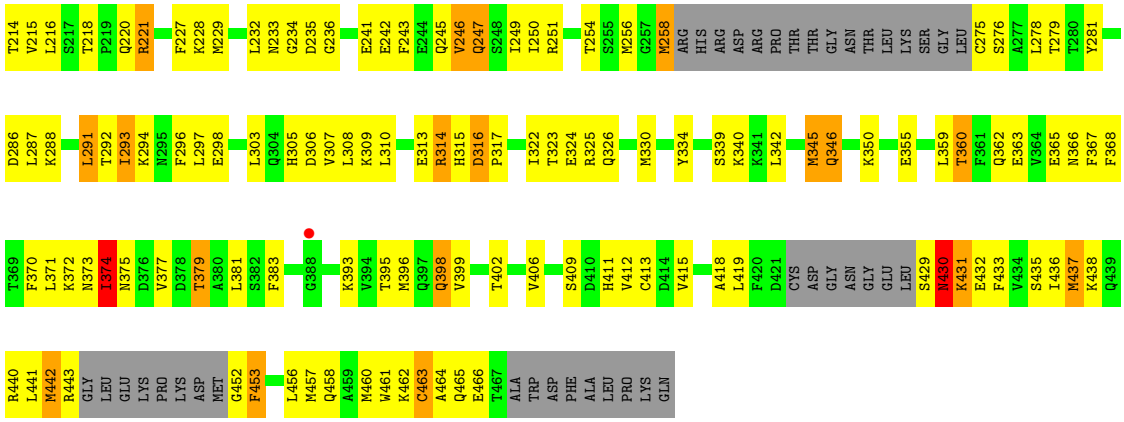
Chain A: 2% 29% 39% 8% 23%




• Molecule 1: Calcium uptake protein 1, mitochondrial

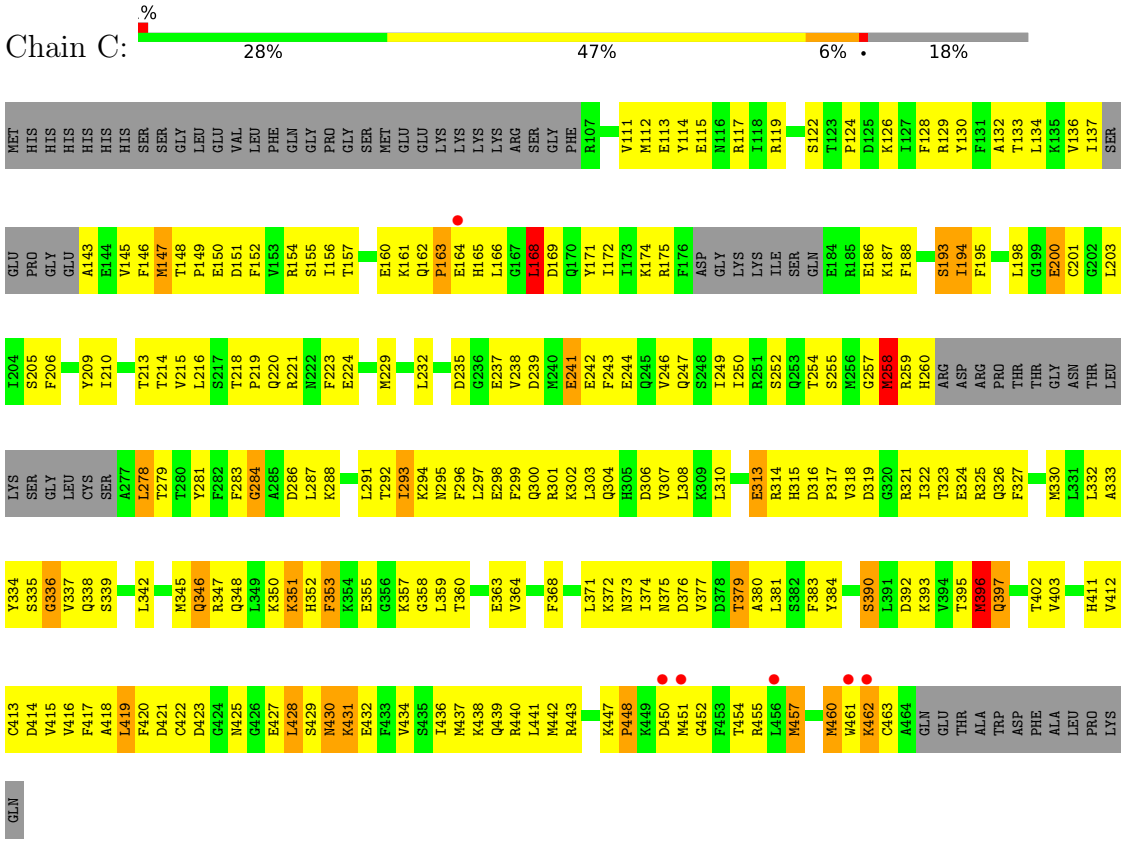
Chain B: 35% 36% 7% • 21%





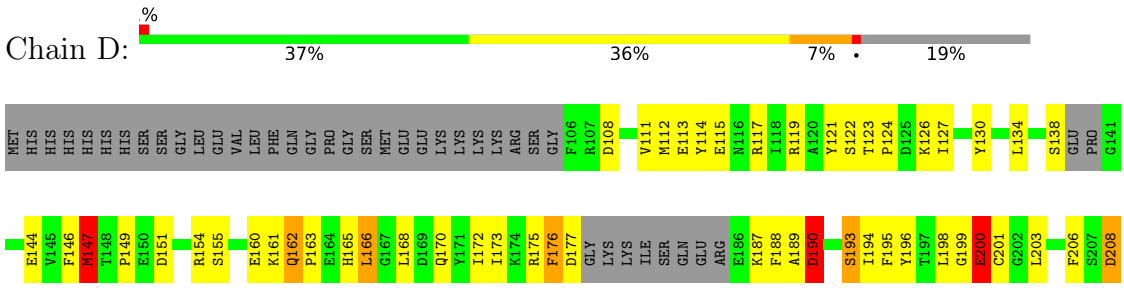

- Molecule 1: Calcium uptake protein 1, mitochondrial

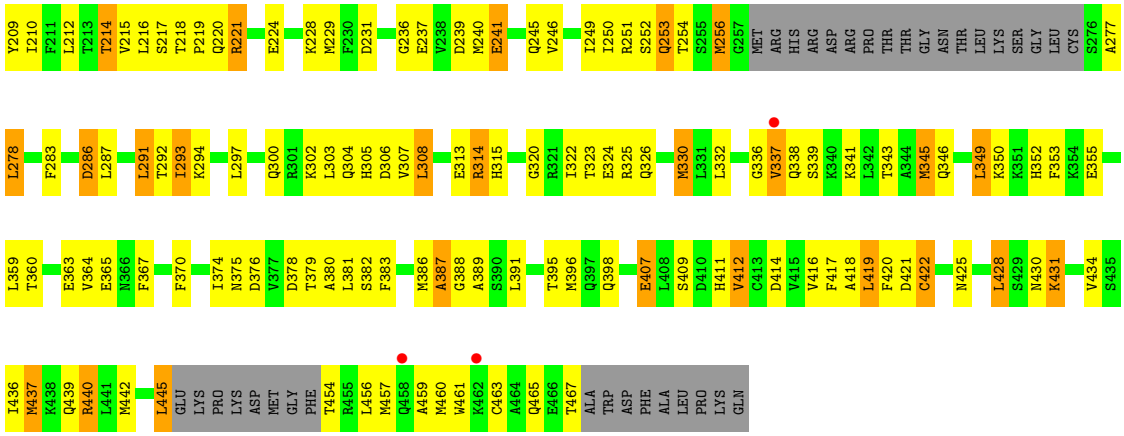
Chain C:




- Molecule 1: Calcium uptake protein 1, mitochondrial

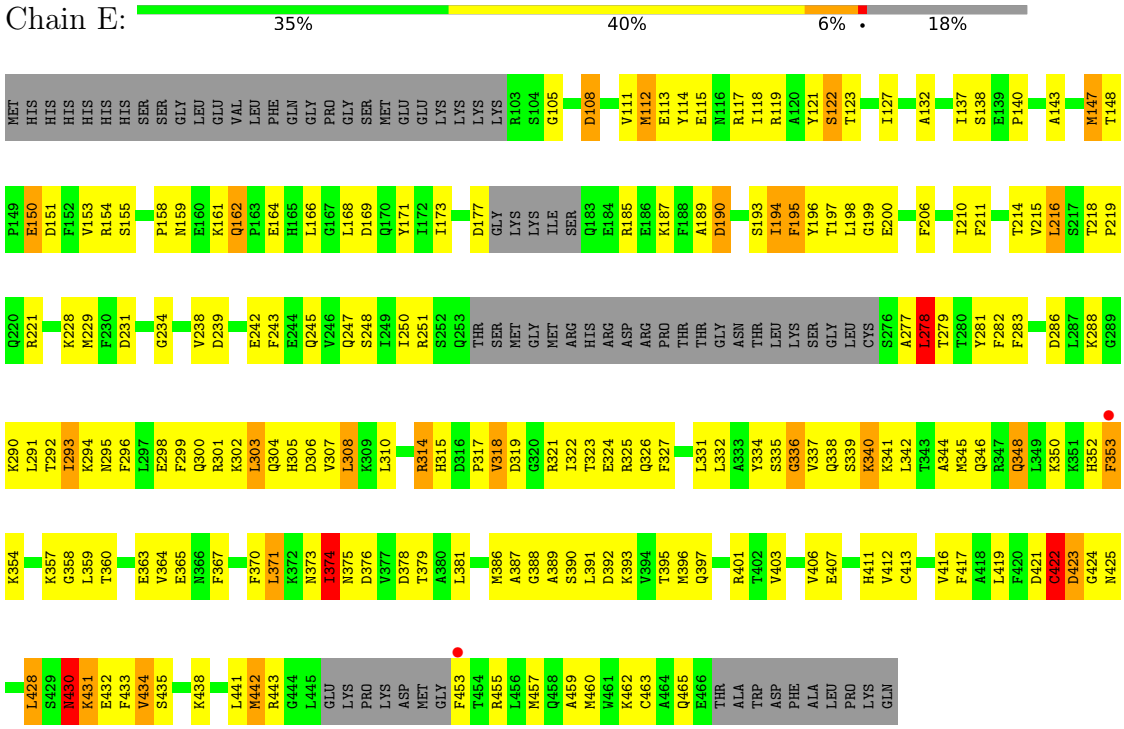
Chain D:





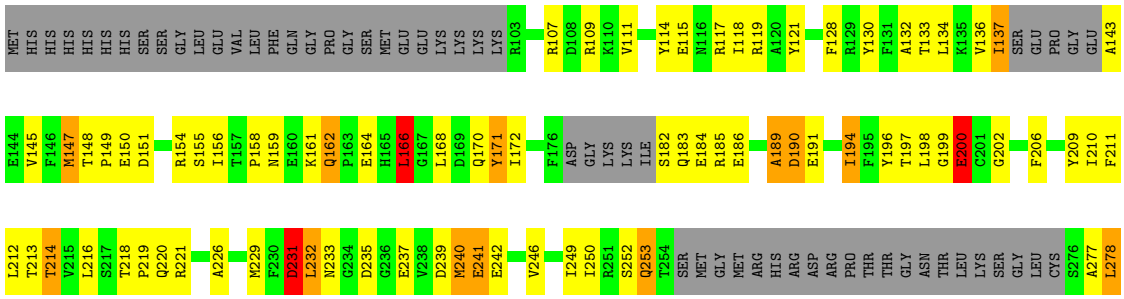

• Molecule 1: Calcium uptake protein 1, mitochondrial

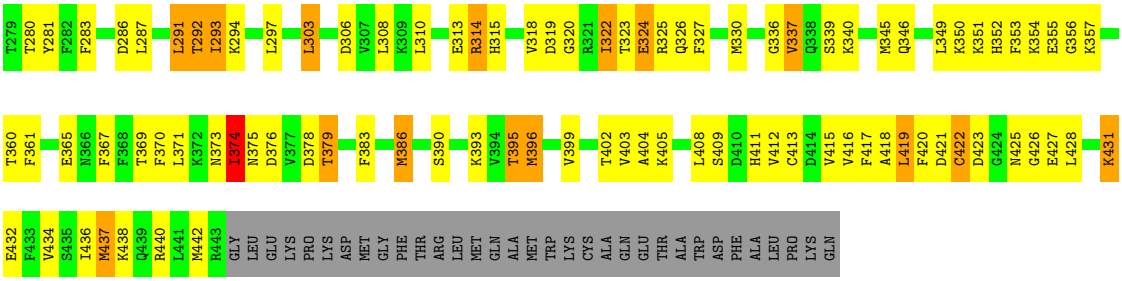
Chain E:




• Molecule 1: Calcium uptake protein 1, mitochondrial

Chain F:




T279 T280 Y281 F282 F283 D286 L287 L291 T292 I293 K294 L297 L303 D306 V307 L308 K309 L310 E313 R314 H315 V318 D319 G320 R321 I322 T323 E324 R325 Q326 F327 M330 G336 V337 Q338 S339 K340 M345 Q346 L349 K350 K351 H352 F353 K354 E355 G356 K357
T360 F361 E365 N366 F367 F368 T369 F370 L371 K372 N373 I374 N375 D376 V377 D378 T379 F383 M386 S390 K393 V394 T395 M396 V399 T402 V403 A404 K405 L408 S409 D410 H411 V412 C413 D414 V415 V416 F417 A418 L419 F420 D421 C422 D423 G424 N425 G426 E427 L428 K431
E432 F433 V434 S435 I436 M437 K438 Q439 R440 L441 M442 R443 GLY LEU GLU LYS PRO LYS ASP MET GLY PHE THR ARG LEU MET GLN ALA MET TRP LYS CYS ALA GLN GLU THR ALA TRP ASP PHE ALA LEU PRO LYS GLN

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 90.88Å 146.82Å 115.87Å<br>90.00° 111.08° 90.00° | Depositor |
| Resolution (Å) | 36.72 – 3.20<br>36.71 – 3.20 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 92.3 (36.72-3.20)<br>92.4 (36.71-3.20) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.31 (at 3.18Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, $R_{free}$ | 0.254 , 0.307<br>0.254 , 0.301 | Depositor<br>DCC |
| $R_{free}$ test set | 2007 reflections (4.31%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 58.1 | Xtriage |
| Anisotropy | 0.235 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.29 , 50.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | 0.026 for h,-k,-h-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.88 | EDS |
| Total number of atoms | 15349 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 69.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

## 5.1 Standard geometry (i)

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 | 0.61 | 10/2517 (0.4%) | 0.66 | 1/3379 (0.0%) |
| 1 | B | 0.67 | 10/2581 (0.4%) | 0.68 | 0/3456 |
| 1 | C | 0.65 | 9/2665 (0.3%) | 0.68 | 1/3577 (0.0%) |
| 1 | D | 0.69 | 8/2649 (0.3%) | 0.73 | 0/3551 |
| 1 | E | 0.62 | 4/2644 (0.2%) | 0.73 | 1/3550 (0.0%) |
| 1 | F | 0.64 | 5/2549 (0.2%) | 0.74 | 2/3418 (0.1%) |
| All | All | 0.65 | 46/15605 (0.3%) | 0.71 | 5/20931 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | B | 0 | 1 |

The worst 5 of 46 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 147 | MET | CG-SD | 9.03 | 2.04 | 1.81 |
| 1 | D | 147 | MET | CG-SD | 8.10 | 2.02 | 1.81 |
| 1 | D | 229 | MET | CG-SD | 7.68 | 2.01 | 1.81 |
| 1 | F | 442 | MET | CG-SD | 7.67 | 2.01 | 1.81 |
| 1 | D | 256 | MET | CG-SD | 7.62 | 2.00 | 1.81 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 448 | PRO | N-CA-CB | 6.02 | 110.52 | 103.30 |
| 1 | F | 356 | GLY | N-CA-C | 5.90 | 127.85 | 113.10 |
| 1 | E | 278 | LEU | CA-CB-CG | 5.53 | 128.02 | 115.30 |
| 1 | F | 166 | LEU | CA-CB-CG | -5.36 | 102.97 | 115.30 |
| 1 | A | 441 | LEU | CA-CB-CG | 5.26 | 127.39 | 115.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 196 | TYR | Sidechain |

## 5.2 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 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 | 2472 | 0 | 2397 | 221 | 0 |
| 1 | B | 2539 | 0 | 2496 | 197 | 0 |
| 1 | C | 2619 | 0 | 2542 | 230 | 0 |
| 1 | D | 2604 | 0 | 2547 | 208 | 0 |
| 1 | E | 2598 | 0 | 2494 | 184 | 1 |
| 1 | F | 2504 | 0 | 2458 | 197 | 1 |
| 2 | A | 4 | 0 | 0 | 0 | 0 |
| 2 | B | 3 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 2 | F | 4 | 0 | 0 | 0 | 0 |
| All | All | 15349 | 0 | 14934 | 1171 | 1 |

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 39.

The worst 5 of 1171 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) |
|---|---|---|---|
| 1:D:147:MET:SD | 1:D:147:MET:CG | 2.02 | 1.48 |
| 1:C:147:MET:CG | 1:C:147:MET:SD | 2.04 | 1.44 |
| 1:C:323:THR:HB | 1:C:326:GLN:HG3 | 1.23 | 1.14 |
| 1:F:323:THR:HB | 1:F:326:GLN:HG3 | 1.23 | 1.14 |
| 1:E:323:THR:HB | 1:E:326:GLN:HG3 | 1.28 | 1.14 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:171:TYR:O | 1:F:357:LYS:NZ[2_756] | 2.10 | 0.10 |

## 5.3 Torsion angles (i)

### 5.3.1 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 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 | 300/401 (75%) | 227 (76%) | 54 (18%) | 19 (6%) | 1 | 10 |
| 1 | B | 304/401 (76%) | 235 (77%) | 53 (17%) | 16 (5%) | 2 | 15 |
| 1 | C | 322/401 (80%) | 248 (77%) | 56 (17%) | 18 (6%) | 2 | 14 |
| 1 | D | 316/401 (79%) | 262 (83%) | 39 (12%) | 15 (5%) | 2 | 17 |
| 1 | E | 322/401 (80%) | 261 (81%) | 47 (15%) | 14 (4%) | 2 | 20 |
| 1 | F | 302/401 (75%) | 237 (78%) | 49 (16%) | 16 (5%) | 2 | 15 |
| All | All | 1866/2406 (78%) | 1470 (79%) | 298 (16%) | 98 (5%) | 2 | 15 |

5 of 98 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 166 | LEU |
| 1 | A | 172 | ILE |
| 1 | A | 354 | LYS |
| 1 | A | 453 | PHE |
| 1 | B | 374 | ILE |

### 5.3.2 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 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 | 259/354 (73%) | 232 (90%) | 27 (10%) | 7 | 28 |
| 1 | B | 273/354 (77%) | 243 (89%) | 30 (11%) | 6 | 26 |
| 1 | C | 274/354 (77%) | 249 (91%) | 25 (9%) | 9 | 34 |
| 1 | D | 278/354 (78%) | 256 (92%) | 22 (8%) | 12 | 43 |
| 1 | E | 269/354 (76%) | 240 (89%) | 29 (11%) | 6 | 27 |
| 1 | F | 270/354 (76%) | 241 (89%) | 29 (11%) | 6 | 27 |
| All | All | 1623/2124 (76%) | 1461 (90%) | 162 (10%) | 7 | 30 |

5 of 162 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 303 | LEU |
| 1 | F | 235 | ASP |
| 1 | E | 340 | LYS |
| 1 | E | 430 | ASN |
| 1 | F | 293 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 300 | GLN |
| 1 | F | 397 | GLN |
| 1 | E | 315 | HIS |
| 1 | E | 439 | GLN |
| 1 | C | 162 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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 | 310/401 (77%) | 0.09 | 7 (2%) | 60 | 47 | 62, 86, 113, 127 | 0 |
| 1 | B | 316/401 (78%) | -0.11 | 2 (0%) | 89 | 83 | 41, 73, 104, 122 | 0 |
| 1 | C | 330/401 (82%) | -0.15 | 6 (1%) | 68 | 55 | 44, 70, 97, 114 | 0 |
| 1 | D | 326/401 (81%) | -0.17 | 3 (0%) | 84 | 75 | 36, 60, 89, 111 | 0 |
| 1 | E | 330/401 (82%) | -0.30 | 2 (0%) | 89 | 83 | 32, 59, 107, 122 | 0 |
| 1 | F | 310/401 (77%) | -0.33 | 0 | 100 | 100 | 36, 58, 95, 112 | 0 |
| All | All | 1922/2406 (79%) | -0.16 | 20 (1%) | 82 | 72 | 32, 69, 104, 127 | 0 |

The worst 5 of 20 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 461 | TRP | 5.1 |
| 1 | C | 462 | LYS | 3.6 |
| 1 | A | 124 | PRO | 3.4 |
| 1 | E | 453 | PHE | 3.1 |
| 1 | C | 456 | LEU | 3.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.