



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:27 AM UTC

PDB ID : 5BW9 / pdb\_00005bw9  
Title : Crystal Structure of Yeast V1-ATPase in the Autoinhibited Form  
Authors : Oot, R.A.; Kane, P.M.; Berry, E.A.; Wilkens, S.  
Deposited on : 2015-06-06  
Resolution : 7.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

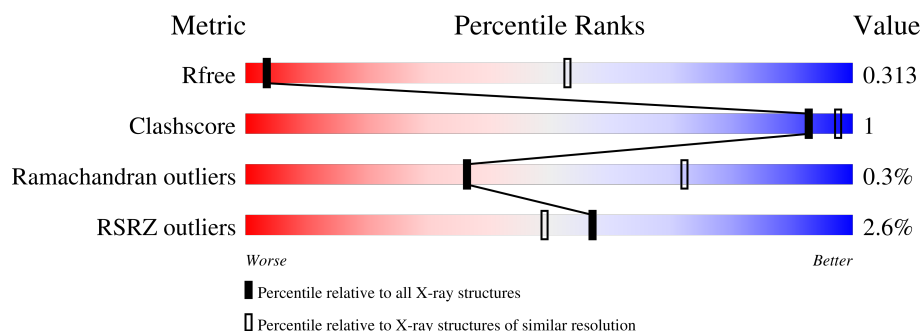
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.00 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1167 (10.00-4.00)                                     |
| Clashscore            | 190562                      | 1007 (9.70-4.04)                                      |
| Ramachandran outliers | 187476                      | 1054 (10.00-4.00)                                     |
| RSRZ outliers         | 180081                      | 1161 (10.00-4.00)                                     |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 617    | <div> <div>3%</div> <div>91%</div> <div>5%</div> <div>.</div> </div> |
| 1   | B     | 617    | <div> <div>2%</div> <div>92%</div> <div>.</div> <div>.</div> </div>  |
| 1   | C     | 617    | <div> <div>3%</div> <div>92%</div> <div>.</div> <div>5%</div> </div> |
| 1   | a     | 617    | <div> <div>5%</div> <div>91%</div> <div>5%</div> <div>.</div> </div> |
| 1   | b     | 617    | <div> <div>%</div> <div>91%</div> <div>.</div> <div>5%</div> </div>  |
| 1   | c     | 617    | <div> <div>2%</div> <div>92%</div> <div>.</div> <div>5%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | D     | 517    |                  |
| 2   | E     | 517    |                  |
| 2   | F     | 517    |                  |
| 2   | d     | 517    |                  |
| 2   | e     | 517    |                  |
| 2   | f     | 517    |                  |
| 3   | H     | 478    |                  |
| 3   | h     | 478    |                  |
| 4   | G     | 256    |                  |
| 4   | g     | 256    |                  |
| 5   | J     | 122    |                  |
| 5   | L     | 122    |                  |
| 5   | N     | 122    |                  |
| 5   | j     | 122    |                  |
| 5   | l     | 122    |                  |
| 5   | n     | 122    |                  |
| 6   | I     | 233    |                  |
| 6   | K     | 233    |                  |
| 6   | M     | 233    |                  |
| 6   | i     | 233    |                  |
| 6   | k     | 233    |                  |
| 6   | m     | 233    |                  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 44760 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 V-type proton ATPase catalytic subunit A.

| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 1   | A     | 591      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2905  | 1723 | 591 | 591 |         |         |       |
| 1   | B     | 594      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2920  | 1732 | 594 | 594 |         |         |       |
| 1   | C     | 589      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2895  | 1717 | 589 | 589 |         |         |       |
| 1   | a     | 591      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2905  | 1723 | 591 | 591 |         |         |       |
| 1   | b     | 589      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2895  | 1717 | 589 | 589 |         |         |       |
| 1   | c     | 586      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2880  | 1708 | 586 | 586 |         |         |       |

- Molecule 2 is a protein called V-type proton ATPase subunit B.

| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 2   | D     | 457      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2250  | 1336 | 457 | 457 |         |         |       |
| 2   | E     | 453      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2231  | 1325 | 453 | 453 |         |         |       |
| 2   | F     | 449      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2211  | 1313 | 449 | 449 |         |         |       |
| 2   | d     | 460      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2265  | 1345 | 460 | 460 |         |         |       |
| 2   | e     | 456      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2245  | 1333 | 456 | 456 |         |         |       |
| 2   | f     | 449      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2212  | 1314 | 449 | 449 |         |         |       |

- Molecule 3 is a protein called V-type proton ATPase subunit H.

| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 3   | H     | 445      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2212  | 1322 | 445 | 445 |         |         |       |
| 3   | h     | 444      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2208  | 1320 | 444 | 444 |         |         |       |

- Molecule 4 is a protein called V-type proton ATPase subunit D.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 4   | G     | 139      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 691   | 413 | 139 | 139 |         |         |       |
| 4   | g     | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 701   | 419 | 141 | 141 |         |         |       |

- Molecule 5 is a protein called V-type proton ATPase subunit G.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | J     | 104      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 514   | 306 | 104 | 104 |         |         |       |
| 5   | L     | 68       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 335   | 199 | 68  | 68  |         |         |       |
| 5   | N     | 81       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 400   | 238 | 81  | 81  |         |         |       |
| 5   | j     | 101      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 499   | 297 | 101 | 101 |         |         |       |
| 5   | l     | 66       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 325   | 193 | 66  | 66  |         |         |       |
| 5   | n     | 58       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 288   | 172 | 58  | 58  |         |         |       |

There are 54 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| J     | -7      | MET      | -      | initiating methionine | UNP P48836 |
| J     | -6      | ASP      | -      | expression tag        | UNP P48836 |
| J     | -5      | TYR      | -      | expression tag        | UNP P48836 |
| J     | -4      | LYS      | -      | expression tag        | UNP P48836 |
| J     | -3      | ASP      | -      | expression tag        | UNP P48836 |
| J     | -2      | ASP      | -      | expression tag        | UNP P48836 |
| J     | -1      | ASP      | -      | expression tag        | UNP P48836 |
| J     | 0       | ASP      | -      | expression tag        | UNP P48836 |
| J     | 1       | LYS      | -      | expression tag        | UNP P48836 |
| L     | -7      | MET      | -      | initiating methionine | UNP P48836 |
| L     | -6      | ASP      | -      | expression tag        | UNP P48836 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| L     | -5      | TYR      | -      | expression tag        | UNP P48836 |
| L     | -4      | LYS      | -      | expression tag        | UNP P48836 |
| L     | -3      | ASP      | -      | expression tag        | UNP P48836 |
| L     | -2      | ASP      | -      | expression tag        | UNP P48836 |
| L     | -1      | ASP      | -      | expression tag        | UNP P48836 |
| L     | 0       | ASP      | -      | expression tag        | UNP P48836 |
| L     | 1       | LYS      | -      | expression tag        | UNP P48836 |
| N     | -7      | MET      | -      | initiating methionine | UNP P48836 |
| N     | -6      | ASP      | -      | expression tag        | UNP P48836 |
| N     | -5      | TYR      | -      | expression tag        | UNP P48836 |
| N     | -4      | LYS      | -      | expression tag        | UNP P48836 |
| N     | -3      | ASP      | -      | expression tag        | UNP P48836 |
| N     | -2      | ASP      | -      | expression tag        | UNP P48836 |
| N     | -1      | ASP      | -      | expression tag        | UNP P48836 |
| N     | 0       | ASP      | -      | expression tag        | UNP P48836 |
| N     | 1       | LYS      | -      | expression tag        | UNP P48836 |
| j     | -7      | MET      | -      | initiating methionine | UNP P48836 |
| j     | -6      | ASP      | -      | expression tag        | UNP P48836 |
| j     | -5      | TYR      | -      | expression tag        | UNP P48836 |
| j     | -4      | LYS      | -      | expression tag        | UNP P48836 |
| j     | -3      | ASP      | -      | expression tag        | UNP P48836 |
| j     | -2      | ASP      | -      | expression tag        | UNP P48836 |
| j     | -1      | ASP      | -      | expression tag        | UNP P48836 |
| j     | 0       | ASP      | -      | expression tag        | UNP P48836 |
| j     | 1       | LYS      | -      | expression tag        | UNP P48836 |
| l     | -7      | MET      | -      | initiating methionine | UNP P48836 |
| l     | -6      | ASP      | -      | expression tag        | UNP P48836 |
| l     | -5      | TYR      | -      | expression tag        | UNP P48836 |
| l     | -4      | LYS      | -      | expression tag        | UNP P48836 |
| l     | -3      | ASP      | -      | expression tag        | UNP P48836 |
| l     | -2      | ASP      | -      | expression tag        | UNP P48836 |
| l     | -1      | ASP      | -      | expression tag        | UNP P48836 |
| l     | 0       | ASP      | -      | expression tag        | UNP P48836 |
| l     | 1       | LYS      | -      | expression tag        | UNP P48836 |
| n     | -7      | MET      | -      | initiating methionine | UNP P48836 |
| n     | -6      | ASP      | -      | expression tag        | UNP P48836 |
| n     | -5      | TYR      | -      | expression tag        | UNP P48836 |
| n     | -4      | LYS      | -      | expression tag        | UNP P48836 |
| n     | -3      | ASP      | -      | expression tag        | UNP P48836 |
| n     | -2      | ASP      | -      | expression tag        | UNP P48836 |
| n     | -1      | ASP      | -      | expression tag        | UNP P48836 |
| n     | 0       | ASP      | -      | expression tag        | UNP P48836 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| n     | 1       | LYS      | -      | expression tag | UNP P48836 |

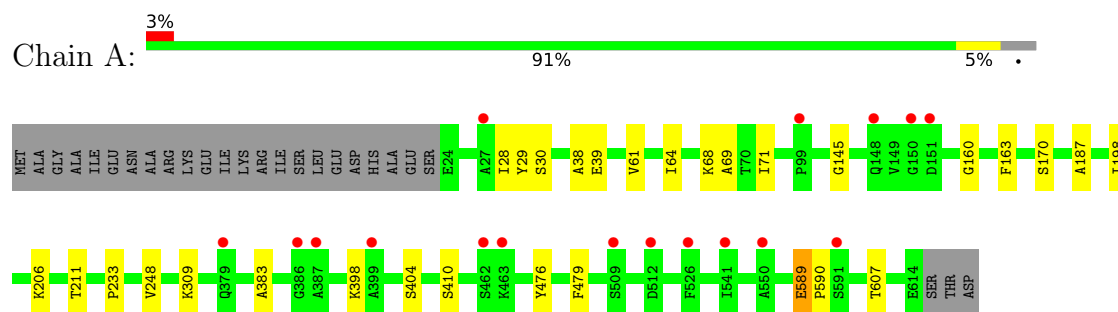
- Molecule 6 is a protein called V-type proton ATPase subunit E.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 6   | I     | 216      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 641 | 216 | 216 |         |         |       |
| 6   | K     | 178      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 883   | 527 | 178 | 178 |         |         |       |
| 6   | M     | 203      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1008  | 602 | 203 | 203 |         |         |       |
| 6   | i     | 217      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1078  | 644 | 217 | 217 |         |         |       |
| 6   | k     | 168      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 833   | 497 | 168 | 168 |         |         |       |
| 6   | m     | 181      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 898   | 536 | 181 | 181 |         |         |       |

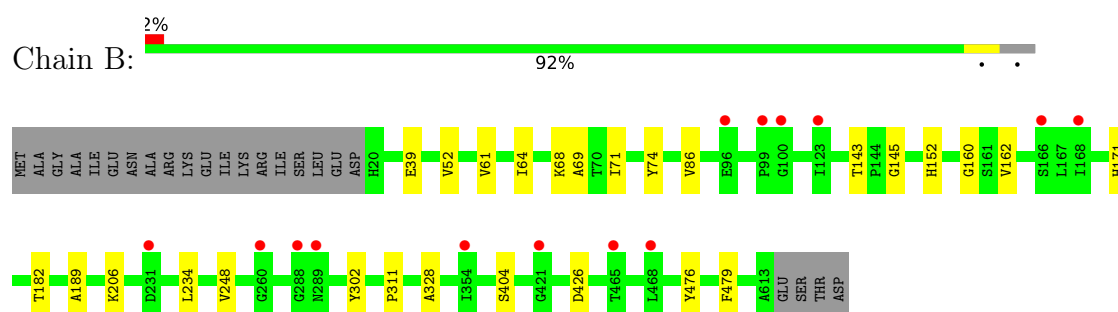
### 3 Residue-property plots [i](#)

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.

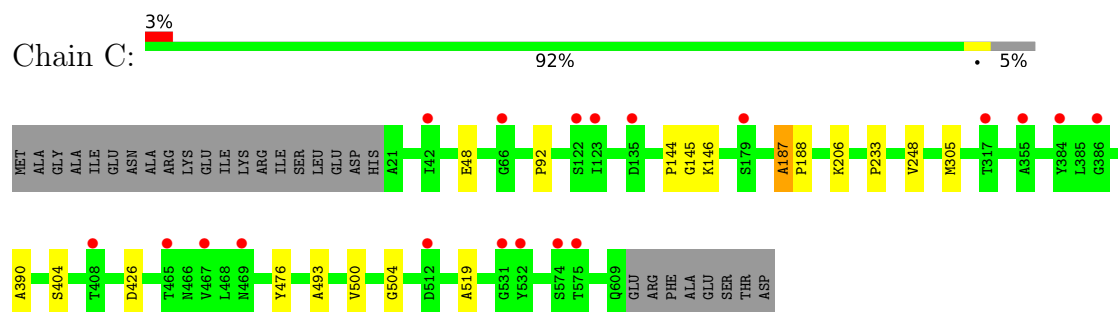
- Molecule 1: V-type proton ATPase catalytic subunit A



- Molecule 1: V-type proton ATPase catalytic subunit A

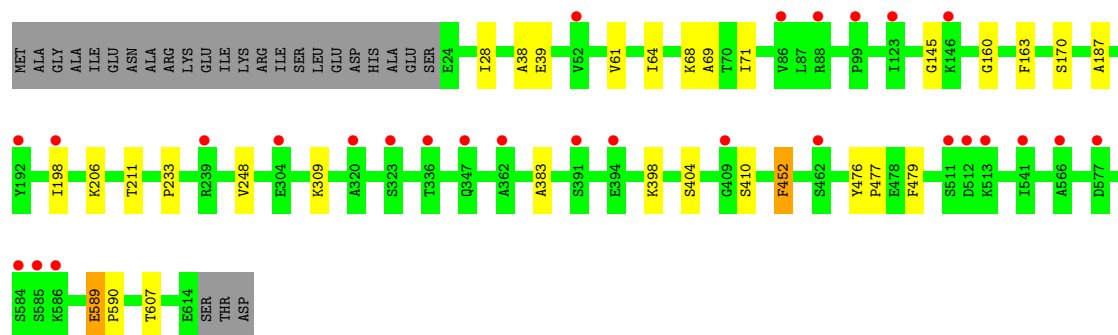


- Molecule 1: V-type proton ATPase catalytic subunit A

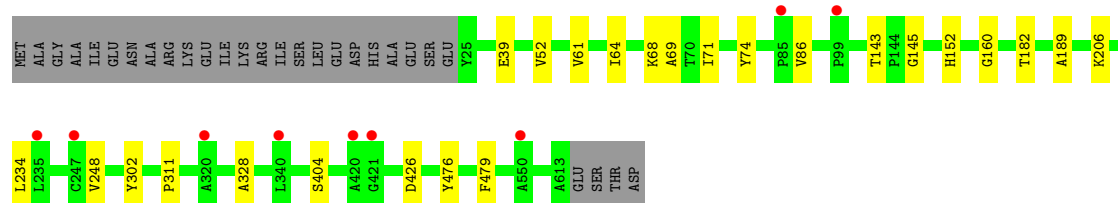


- Molecule 1: V-type proton ATPase catalytic subunit A

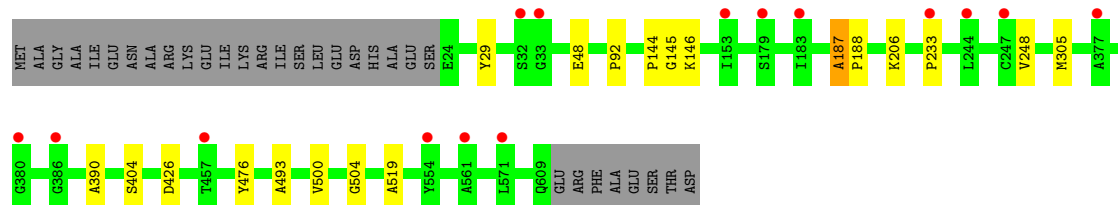




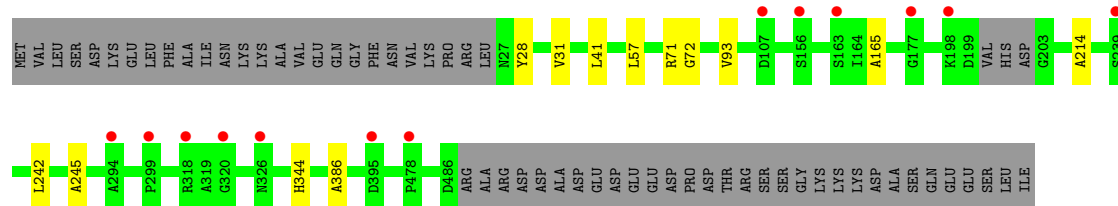
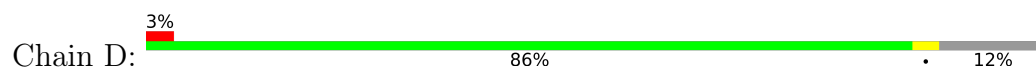
- Molecule 1: V-type proton ATPase catalytic subunit A



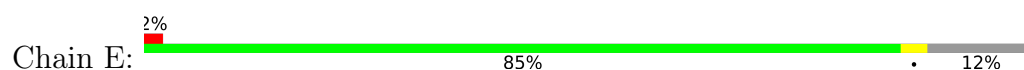
- Molecule 1: V-type proton ATPase catalytic subunit A

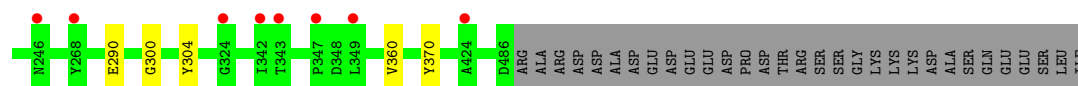


- Molecule 2: V-type proton ATPase subunit B

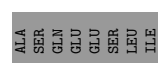
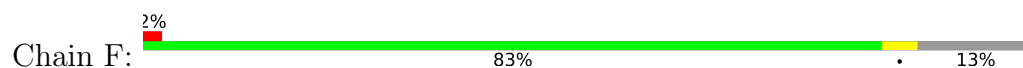


- Molecule 2: V-type proton ATPase subunit B

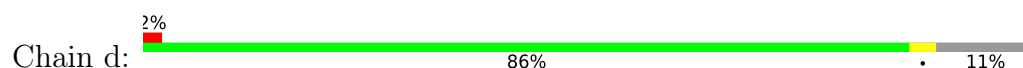




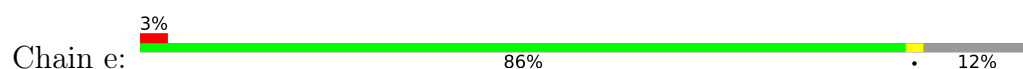
• Molecule 2: V-type proton ATPase subunit B



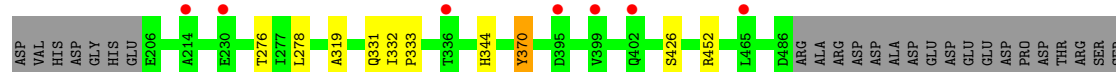
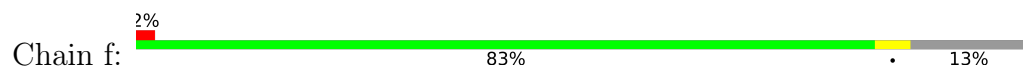
• Molecule 2: V-type proton ATPase subunit B



• Molecule 2: V-type proton ATPase subunit B

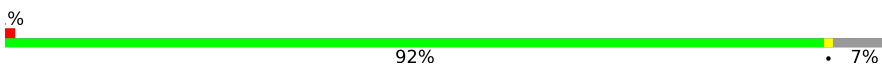


• Molecule 2: V-type proton ATPase subunit B



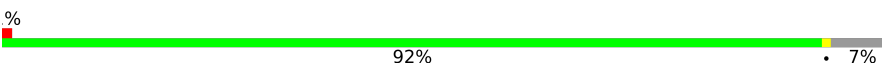
GLY  
LYS  
LYS  
LYS  
ASP  
SER  
GLN  
GLU  
GLU  
SER  
LEU  
ILE

• Molecule 3: V-type proton ATPase subunit H

Chain H:  92% 7%

MET G2 S10 K53 LYS ASN ILE ILE GLY ASP GLY LEU SER SER SER SER ASN ASN ALA HIS SER SER GLY PHE K71 G134 D223 SER GLN LEU LEU ALA THR ARG ILE VAL ALA THR ASN SER ASN H237 E352 L353 T354 S355 D365 Y475 T476 PHE LYS

• Molecule 3: V-type proton ATPase subunit H

Chain h:  92% 7%

MET GLY A3 K53 LYS ASN ILE ILE GLY ASP GLY LEU SER SER SER SER ASN ASN ALA HIS SER SER GLY PHE K71 Q152 D223 SER GLN LEU LEU ALA THR ARG ILE VAL ALA THR ASN ASN H237 C297 R301 E352 L353 T354 S355 G378 I473 G474 Y475 T476 PHE LYS

• Molecule 4: V-type proton ATPase subunit D

Chain G:  54% 46%

MET SER ILE ASP GLY ASN ARG GLU VAL F9 Q62 THR ALA ALA PHE SER LEU LEU GLY THR ALA ARG PHE ASP ILE THR LEU THR GLN ARG A135 I138 V147 H175 K219 GLU MET LYS LEU SER LYS ARG ASP ALA ARG ALA GLN ASP ALA SER GLU VAL ALA ASP GLU GLU GLN PRO VAL TYR LEU SER GLN PHE THR LEU VAL

TYR ILE ASP PRO GLU ILE ASP PHE ARG LEU THR GLY LEU LEU GLY ARG GLY GLN VAL VAL GLN ARG A135 I138 V147 H175 K219 GLU MET LYS LEU SER LYS ARG ASP ALA ARG ALA GLN ASP ALA SER GLU VAL ALA ASP GLU GLU GLN PRO VAL TYR LEU SER GLN PHE THR LEU VAL

ALA  
ASP  
GLN  
GLU  
ASP  
ASP  
VAL  
ILE  
PHE

• Molecule 4: V-type proton ATPase subunit D

Chain g:  55% 45%

MET SER TYR ILE ASP GLY ASN ARG GLU VAL F9 M61 GLN THR ALA ALA PHE SER LEU LEU GLY THR ALA ARG PHE ASP ILE THR LEU THR GLN ARG A135 I138 V147 H175 K219 GLU MET LYS LEU SER LYS ARG ASP ALA ARG ALA GLN ASP ALA SER GLU VAL ALA ASP GLU GLU GLN PRO VAL TYR LEU SER GLN PHE THR LEU VAL

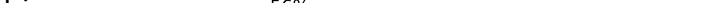
SER TYR ILE ASP PRO GLU ILE ASP PHE ARG LEU THR GLY LEU LEU GLY ARG GLY GLN VAL VAL GLN ARG ALA LYS ILE Y139 H175 D226 ARG ALA GLU GLN GLN ASP ALA GLU PHE VAL ALA ASP GLU GLU PRO GLN GLY GLU THR LEU VAL VAL ALA ASP GLN GLU ASP

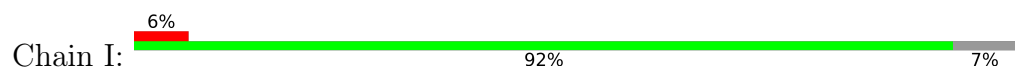
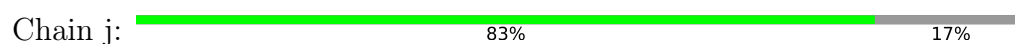
VAL  
ILE  
PHE

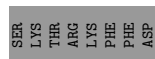
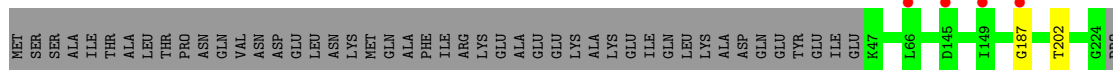
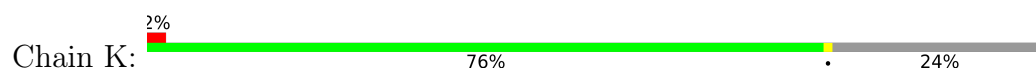
• Molecule 5: V-type proton ATPase subunit G

Chain J:  85% 15%

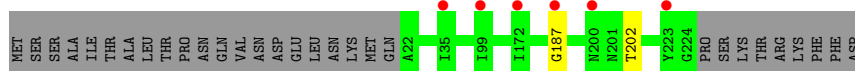
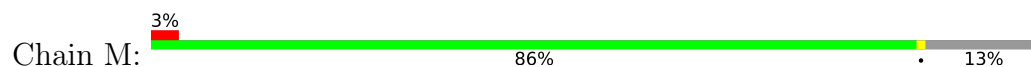
MET ASP TYR LYS ASP ASP ASP LYS SER Q3 I43 I103 S106 ALA GLU VAL HIS ILE ASN ALA LEU

- Chain L:  2% 56% 44%

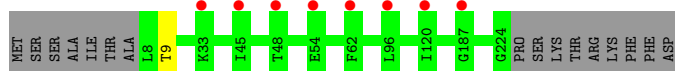




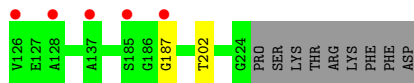
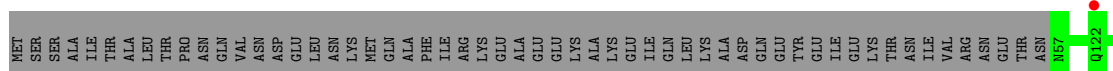
- Molecule 6: V-type proton ATPase subunit E



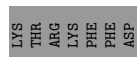
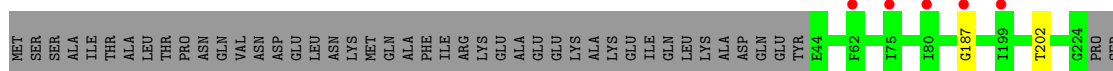
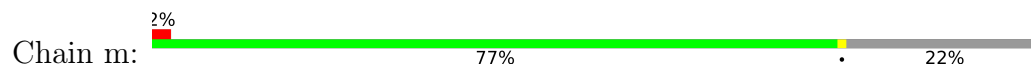
- Molecule 6: V-type proton ATPase subunit E



- Molecule 6: V-type proton ATPase subunit E



- Molecule 6: V-type proton ATPase subunit E



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 468.48Å 159.74Å 245.04Å<br>90.00° 113.88° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 40.10 – 7.00<br>40.10 – 7.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (40.10-7.00)<br>89.8 (40.10-7.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.19                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.75 (at 7.33Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: dev_1957)                            | Depositor        |
| R, $R_{free}$                                                           | 0.260 , 0.309<br>0.268 , 0.313                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (7.66%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 321.6                                                       | Xtriage          |
| Anisotropy                                                              | 0.269                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.39 , 999.0                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.81                                                        | EDS              |
| Total number of atoms                                                   | 44760                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 290.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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     | 0.30         | 0/2904  | 0.90        | 8/4034 (0.2%)   |
| 1   | B     | 0.29         | 0/2919  | 0.87        | 9/4055 (0.2%)   |
| 1   | C     | 0.30         | 0/2894  | 0.87        | 9/4020 (0.2%)   |
| 1   | a     | 0.30         | 0/2904  | 0.91        | 12/4034 (0.3%)  |
| 1   | b     | 0.30         | 0/2894  | 0.87        | 9/4020 (0.2%)   |
| 1   | c     | 0.30         | 0/2879  | 0.86        | 9/3999 (0.2%)   |
| 2   | D     | 0.30         | 0/2248  | 0.85        | 4/3123 (0.1%)   |
| 2   | E     | 0.30         | 0/2229  | 0.85        | 6/3097 (0.2%)   |
| 2   | F     | 0.29         | 0/2209  | 0.84        | 5/3069 (0.2%)   |
| 2   | d     | 0.30         | 0/2264  | 0.85        | 6/3147 (0.2%)   |
| 2   | e     | 0.30         | 0/2243  | 0.86        | 6/3116 (0.2%)   |
| 2   | f     | 0.30         | 0/2210  | 0.84        | 7/3071 (0.2%)   |
| 3   | H     | 0.31         | 0/2209  | 0.84        | 2/3080 (0.1%)   |
| 3   | h     | 0.31         | 0/2205  | 0.84        | 2/3075 (0.1%)   |
| 4   | G     | 0.30         | 0/689   | 0.80        | 0/959           |
| 4   | g     | 0.30         | 0/699   | 0.78        | 0/973           |
| 5   | J     | 0.29         | 0/513   | 0.79        | 0/713           |
| 5   | L     | 0.30         | 0/334   | 0.81        | 0/463           |
| 5   | N     | 0.30         | 0/399   | 0.80        | 0/554           |
| 5   | j     | 0.29         | 0/498   | 0.78        | 0/692           |
| 5   | l     | 0.30         | 0/324   | 0.81        | 0/449           |
| 5   | n     | 0.29         | 0/286   | 0.75        | 0/396           |
| 6   | I     | 0.29         | 0/1072  | 0.83        | 2/1495 (0.1%)   |
| 6   | K     | 0.29         | 0/882   | 0.83        | 0/1229          |
| 6   | M     | 0.29         | 0/1007  | 0.78        | 0/1404          |
| 6   | i     | 0.29         | 0/1077  | 0.83        | 2/1502 (0.1%)   |
| 6   | k     | 0.29         | 0/832   | 0.83        | 0/1159          |
| 6   | m     | 0.29         | 0/897   | 0.79        | 0/1250          |
| All | All   | 0.30         | 0/44720 | 0.85        | 98/62178 (0.2%) |

There are no bond length outliers.

All (98) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | a     | 589 | GLU  | CA-C-N  | 11.55 | 134.27      | 119.84   |
| 1   | a     | 589 | GLU  | C-N-CA  | 11.55 | 134.27      | 119.84   |
| 1   | A     | 589 | GLU  | CA-C-N  | 11.10 | 133.71      | 119.84   |
| 1   | A     | 589 | GLU  | C-N-CA  | 11.10 | 133.71      | 119.84   |
| 1   | a     | 479 | PHE  | CA-C-N  | 9.61  | 130.27      | 119.32   |
| 1   | a     | 479 | PHE  | C-N-CA  | 9.61  | 130.27      | 119.32   |
| 1   | A     | 479 | PHE  | CA-C-N  | 9.54  | 130.20      | 119.32   |
| 1   | A     | 479 | PHE  | C-N-CA  | 9.54  | 130.20      | 119.32   |
| 1   | C     | 187 | ALA  | CA-C-N  | 8.01  | 129.86      | 119.84   |
| 1   | C     | 187 | ALA  | C-N-CA  | 8.01  | 129.86      | 119.84   |
| 1   | c     | 187 | ALA  | CA-C-N  | 8.01  | 129.85      | 119.84   |
| 1   | c     | 187 | ALA  | C-N-CA  | 8.01  | 129.85      | 119.84   |
| 1   | B     | 479 | PHE  | CA-C-N  | 7.96  | 127.88      | 119.05   |
| 1   | B     | 479 | PHE  | C-N-CA  | 7.96  | 127.88      | 119.05   |
| 1   | b     | 479 | PHE  | CA-C-N  | 7.94  | 127.86      | 119.05   |
| 1   | b     | 479 | PHE  | C-N-CA  | 7.94  | 127.86      | 119.05   |
| 6   | I     | 9   | THR  | CA-C-N  | 7.60  | 127.31      | 119.56   |
| 6   | I     | 9   | THR  | C-N-CA  | 7.60  | 127.31      | 119.56   |
| 6   | i     | 9   | THR  | CA-C-N  | 7.56  | 127.27      | 119.56   |
| 6   | i     | 9   | THR  | C-N-CA  | 7.56  | 127.27      | 119.56   |
| 1   | a     | 476 | TYR  | CA-C-N  | 6.53  | 128.00      | 119.84   |
| 1   | a     | 476 | TYR  | C-N-CA  | 6.53  | 128.00      | 119.84   |
| 1   | B     | 476 | TYR  | CA-C-N  | 6.51  | 126.69      | 120.31   |
| 1   | B     | 476 | TYR  | C-N-CA  | 6.51  | 126.69      | 120.31   |
| 1   | b     | 476 | TYR  | CA-C-N  | 6.46  | 126.64      | 120.31   |
| 1   | b     | 476 | TYR  | C-N-CA  | 6.46  | 126.64      | 120.31   |
| 2   | f     | 57  | LEU  | CA-C-N  | 6.42  | 126.04      | 119.56   |
| 2   | f     | 57  | LEU  | C-N-CA  | 6.42  | 126.04      | 119.56   |
| 2   | F     | 57  | LEU  | CA-C-N  | 6.32  | 125.94      | 119.56   |
| 2   | F     | 57  | LEU  | C-N-CA  | 6.32  | 125.94      | 119.56   |
| 3   | H     | 353 | LEU  | CA-C-N  | 5.96  | 132.44      | 121.70   |
| 3   | H     | 353 | LEU  | C-N-CA  | 5.96  | 132.44      | 121.70   |
| 3   | h     | 353 | LEU  | CA-C-N  | 5.95  | 132.42      | 121.70   |
| 3   | h     | 353 | LEU  | C-N-CA  | 5.95  | 132.42      | 121.70   |
| 1   | C     | 404 | SER  | CA-C-N  | 5.87  | 126.28      | 119.47   |
| 1   | C     | 404 | SER  | C-N-CA  | 5.87  | 126.28      | 119.47   |
| 2   | F     | 426 | SER  | CB-CA-C | -5.85 | 109.85      | 116.63   |
| 1   | c     | 404 | SER  | CA-C-N  | 5.83  | 126.23      | 119.47   |
| 1   | c     | 404 | SER  | C-N-CA  | 5.83  | 126.23      | 119.47   |
| 2   | f     | 426 | SER  | CB-CA-C | -5.78 | 109.93      | 116.63   |
| 2   | F     | 344 | HIS  | CA-C-N  | 5.63  | 125.74      | 119.32   |
| 2   | F     | 344 | HIS  | C-N-CA  | 5.63  | 125.74      | 119.32   |
| 1   | C     | 426 | ASP  | CA-C-N  | 5.58  | 125.42      | 119.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 426 | ASP  | C-N-CA  | 5.58  | 125.42      | 119.28   |
| 1   | A     | 206 | LYS  | CB-CA-C | -5.58 | 110.16      | 116.63   |
| 1   | a     | 206 | LYS  | CB-CA-C | -5.56 | 110.18      | 116.63   |
| 2   | f     | 344 | HIS  | CA-C-N  | 5.56  | 125.66      | 119.32   |
| 2   | f     | 344 | HIS  | C-N-CA  | 5.56  | 125.66      | 119.32   |
| 1   | b     | 426 | ASP  | CA-C-N  | 5.54  | 125.64      | 119.32   |
| 1   | b     | 426 | ASP  | C-N-CA  | 5.54  | 125.64      | 119.32   |
| 1   | b     | 404 | SER  | CA-C-N  | 5.54  | 125.89      | 119.47   |
| 1   | b     | 404 | SER  | C-N-CA  | 5.54  | 125.89      | 119.47   |
| 1   | B     | 404 | SER  | CA-C-N  | 5.52  | 125.88      | 119.47   |
| 1   | B     | 404 | SER  | C-N-CA  | 5.52  | 125.88      | 119.47   |
| 1   | B     | 426 | ASP  | CA-C-N  | 5.52  | 125.62      | 119.32   |
| 1   | B     | 426 | ASP  | C-N-CA  | 5.52  | 125.62      | 119.32   |
| 1   | c     | 426 | ASP  | CA-C-N  | 5.52  | 125.36      | 119.28   |
| 1   | c     | 426 | ASP  | C-N-CA  | 5.52  | 125.36      | 119.28   |
| 2   | e     | 57  | LEU  | CA-C-N  | 5.48  | 125.00      | 119.19   |
| 2   | e     | 57  | LEU  | C-N-CA  | 5.48  | 125.00      | 119.19   |
| 2   | E     | 57  | LEU  | CA-C-N  | 5.47  | 124.98      | 119.19   |
| 2   | E     | 57  | LEU  | C-N-CA  | 5.47  | 124.98      | 119.19   |
| 1   | C     | 206 | LYS  | CB-CA-C | -5.46 | 110.30      | 116.63   |
| 1   | b     | 206 | LYS  | CB-CA-C | -5.45 | 110.31      | 116.63   |
| 2   | d     | 57  | LEU  | CA-C-N  | 5.44  | 125.27      | 119.28   |
| 2   | d     | 57  | LEU  | C-N-CA  | 5.44  | 125.27      | 119.28   |
| 1   | c     | 206 | LYS  | CB-CA-C | -5.44 | 110.32      | 116.63   |
| 2   | E     | 140 | ASN  | CA-C-N  | 5.43  | 125.51      | 119.32   |
| 2   | E     | 140 | ASN  | C-N-CA  | 5.43  | 125.51      | 119.32   |
| 1   | A     | 404 | SER  | CA-C-N  | 5.43  | 125.51      | 119.32   |
| 1   | A     | 404 | SER  | C-N-CA  | 5.43  | 125.51      | 119.32   |
| 1   | B     | 206 | LYS  | CB-CA-C | -5.43 | 110.33      | 116.63   |
| 1   | a     | 404 | SER  | CA-C-N  | 5.41  | 125.49      | 119.32   |
| 1   | a     | 404 | SER  | C-N-CA  | 5.41  | 125.49      | 119.32   |
| 2   | D     | 57  | LEU  | CA-C-N  | 5.39  | 125.21      | 119.28   |
| 2   | D     | 57  | LEU  | C-N-CA  | 5.39  | 125.21      | 119.28   |
| 2   | e     | 140 | ASN  | CA-C-N  | 5.37  | 125.44      | 119.32   |
| 2   | e     | 140 | ASN  | C-N-CA  | 5.37  | 125.44      | 119.32   |
| 2   | D     | 344 | HIS  | CA-C-N  | 5.23  | 125.03      | 119.28   |
| 2   | D     | 344 | HIS  | C-N-CA  | 5.23  | 125.03      | 119.28   |
| 1   | a     | 607 | THR  | N-CA-C  | -5.22 | 105.59      | 111.28   |
| 1   | A     | 607 | THR  | N-CA-C  | -5.22 | 105.59      | 111.28   |
| 2   | d     | 344 | HIS  | CA-C-N  | 5.21  | 125.02      | 119.28   |
| 2   | d     | 344 | HIS  | C-N-CA  | 5.21  | 125.02      | 119.28   |
| 1   | a     | 452 | PHE  | CA-C-N  | 5.11  | 125.40      | 119.93   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | a     | 452 | PHE  | C-N-CA | 5.11 | 125.40      | 119.93   |
| 1   | c     | 476 | TYR  | CA-C-N | 5.11 | 126.23      | 119.84   |
| 1   | c     | 476 | TYR  | C-N-CA | 5.11 | 126.23      | 119.84   |
| 1   | C     | 476 | TYR  | CA-C-N | 5.08 | 126.19      | 119.84   |
| 1   | C     | 476 | TYR  | C-N-CA | 5.08 | 126.19      | 119.84   |
| 2   | f     | 370 | TYR  | CA-C-N | 5.04 | 125.57      | 120.38   |
| 2   | f     | 370 | TYR  | C-N-CA | 5.04 | 125.57      | 120.38   |
| 2   | e     | 370 | TYR  | CA-C-N | 5.04 | 125.57      | 120.38   |
| 2   | e     | 370 | TYR  | C-N-CA | 5.04 | 125.57      | 120.38   |
| 2   | E     | 370 | TYR  | CA-C-N | 5.03 | 125.56      | 120.38   |
| 2   | E     | 370 | TYR  | C-N-CA | 5.03 | 125.56      | 120.38   |
| 2   | d     | 371 | PRO  | CA-C-N | 5.01 | 126.10      | 119.84   |
| 2   | d     | 371 | PRO  | C-N-CA | 5.01 | 126.10      | 119.84   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 2905  | 0        | 1339     | 12      | 0            |
| 1   | B     | 2920  | 0        | 1348     | 11      | 0            |
| 1   | C     | 2895  | 0        | 1335     | 5       | 0            |
| 1   | a     | 2905  | 0        | 1339     | 10      | 0            |
| 1   | b     | 2895  | 0        | 1335     | 10      | 0            |
| 1   | c     | 2880  | 0        | 1326     | 6       | 0            |
| 2   | D     | 2250  | 0        | 1015     | 7       | 0            |
| 2   | E     | 2231  | 0        | 1006     | 7       | 0            |
| 2   | F     | 2211  | 0        | 999      | 8       | 0            |
| 2   | d     | 2265  | 0        | 1022     | 5       | 0            |
| 2   | e     | 2245  | 0        | 1013     | 6       | 0            |
| 2   | f     | 2212  | 0        | 998      | 9       | 0            |
| 3   | H     | 2212  | 0        | 951      | 2       | 0            |
| 3   | h     | 2208  | 0        | 948      | 2       | 0            |
| 4   | G     | 691   | 0        | 311      | 0       | 0            |
| 4   | g     | 701   | 0        | 312      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | J     | 514   | 0        | 248      | 0       | 0            |
| 5   | L     | 335   | 0        | 160      | 0       | 0            |
| 5   | N     | 400   | 0        | 189      | 0       | 0            |
| 5   | j     | 499   | 0        | 243      | 0       | 0            |
| 5   | l     | 325   | 0        | 150      | 0       | 0            |
| 5   | n     | 288   | 0        | 136      | 0       | 0            |
| 6   | I     | 1073  | 0        | 481      | 0       | 0            |
| 6   | K     | 883   | 0        | 394      | 1       | 0            |
| 6   | M     | 1008  | 0        | 456      | 1       | 0            |
| 6   | i     | 1078  | 0        | 483      | 0       | 0            |
| 6   | k     | 833   | 0        | 374      | 1       | 0            |
| 6   | m     | 898   | 0        | 400      | 1       | 0            |
| All | All   | 44760 | 0        | 20311    | 97      | 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 1.

All (97) 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:H:353:LEU:H   | 3:H:354:THR:C   | 1.97                     | 0.73              |
| 3:H:352:GLU:HA  | 3:H:355:SER:HA  | 1.72                     | 0.72              |
| 3:h:353:LEU:H   | 3:h:354:THR:C   | 1.97                     | 0.71              |
| 3:h:352:GLU:HA  | 3:h:355:SER:HA  | 1.73                     | 0.69              |
| 2:d:28:TYR:H    | 2:d:93:VAL:H    | 1.39                     | 0.69              |
| 2:D:28:TYR:H    | 2:D:93:VAL:H    | 1.39                     | 0.68              |
| 1:a:383:ALA:HB1 | 2:e:290:GLU:HA  | 1.80                     | 0.63              |
| 2:D:31:VAL:HA   | 2:D:41:LEU:HA   | 1.80                     | 0.63              |
| 6:m:187:GLY:HA3 | 6:m:202:THR:HA  | 1.80                     | 0.63              |
| 6:M:187:GLY:HA3 | 6:M:202:THR:HA  | 1.80                     | 0.63              |
| 1:C:390:ALA:HB1 | 2:D:245:ALA:HB1 | 1.80                     | 0.62              |
| 2:d:31:VAL:HA   | 2:d:41:LEU:HA   | 1.81                     | 0.61              |
| 6:k:187:GLY:HA3 | 6:k:202:THR:HA  | 1.85                     | 0.59              |
| 6:K:187:GLY:HA3 | 6:K:202:THR:HA  | 1.85                     | 0.57              |
| 1:A:29:TYR:O    | 2:D:72:GLY:N    | 2.37                     | 0.57              |
| 2:f:51:GLU:HA   | 2:f:99:SER:HA   | 1.87                     | 0.56              |
| 2:F:51:GLU:HA   | 2:F:99:SER:HA   | 1.87                     | 0.56              |
| 2:F:319:ALA:HB2 | 2:F:331:GLN:H   | 1.71                     | 0.56              |
| 1:B:302:TYR:HA  | 1:B:311:PRO:HA  | 1.88                     | 0.55              |
| 2:f:319:ALA:HB2 | 2:f:331:GLN:H   | 1.71                     | 0.55              |
| 1:b:302:TYR:HA  | 1:b:311:PRO:HA  | 1.88                     | 0.55              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:145:GLY:H   | 1:A:160:GLY:HA2 | 1.73                     | 0.54              |
| 1:A:28:ILE:HA   | 1:A:38:ALA:HA   | 1.90                     | 0.54              |
| 1:b:234:LEU:H   | 1:b:248:VAL:HA  | 1.73                     | 0.54              |
| 1:B:145:GLY:H   | 1:B:160:GLY:HA2 | 1.73                     | 0.54              |
| 1:a:145:GLY:H   | 1:a:160:GLY:HA2 | 1.73                     | 0.54              |
| 1:a:233:PRO:HA  | 1:a:248:VAL:HA  | 1.90                     | 0.54              |
| 1:a:28:ILE:HA   | 1:a:38:ALA:HA   | 1.90                     | 0.53              |
| 1:b:145:GLY:H   | 1:b:160:GLY:HA2 | 1.73                     | 0.53              |
| 1:B:234:LEU:H   | 1:B:248:VAL:HA  | 1.73                     | 0.53              |
| 1:c:48:GLU:HA   | 1:c:92:PRO:HA   | 1.89                     | 0.53              |
| 1:C:48:GLU:HA   | 1:C:92:PRO:HA   | 1.89                     | 0.53              |
| 1:B:64:ILE:HA   | 1:B:69:ALA:HA   | 1.91                     | 0.53              |
| 2:e:300:GLY:N   | 2:e:304:TYR:O   | 2.34                     | 0.53              |
| 1:b:52:VAL:HA   | 1:b:86:VAL:HA   | 1.91                     | 0.53              |
| 1:A:233:PRO:HA  | 1:A:248:VAL:HA  | 1.90                     | 0.53              |
| 1:b:64:ILE:HA   | 1:b:69:ALA:HA   | 1.91                     | 0.52              |
| 2:F:154:GLY:O   | 2:F:452:ARG:N   | 2.40                     | 0.51              |
| 1:B:52:VAL:HA   | 1:B:86:VAL:HA   | 1.91                     | 0.50              |
| 2:d:165:ALA:HB2 | 2:d:386:ALA:HB2 | 1.93                     | 0.50              |
| 2:D:165:ALA:HB2 | 2:D:386:ALA:HB2 | 1.93                     | 0.49              |
| 2:E:300:GLY:N   | 2:E:304:TYR:O   | 2.34                     | 0.49              |
| 2:f:32:SER:H    | 2:f:41:LEU:HA   | 1.77                     | 0.49              |
| 2:F:32:SER:H    | 2:F:41:LEU:HA   | 1.77                     | 0.49              |
| 1:B:39:GLU:HA   | 1:B:68:LYS:HA   | 1.95                     | 0.49              |
| 1:a:39:GLU:HA   | 1:a:68:LYS:HA   | 1.94                     | 0.49              |
| 2:f:154:GLY:O   | 2:f:452:ARG:N   | 2.40                     | 0.49              |
| 1:b:39:GLU:HA   | 1:b:68:LYS:HA   | 1.95                     | 0.49              |
| 1:A:39:GLU:HA   | 1:A:68:LYS:HA   | 1.94                     | 0.48              |
| 2:E:51:GLU:HA   | 2:E:99:SER:HA   | 1.95                     | 0.48              |
| 2:e:51:GLU:HA   | 2:e:99:SER:HA   | 1.96                     | 0.48              |
| 1:b:152:HIS:HA  | 1:b:182:THR:HA  | 1.96                     | 0.48              |
| 1:B:74:TYR:HA   | 1:B:328:ALA:HB3 | 1.96                     | 0.48              |
| 1:A:30:SER:HA   | 2:D:71:ARG:HA   | 1.96                     | 0.48              |
| 2:f:44:VAL:N    | 2:f:73:ASP:O    | 2.37                     | 0.47              |
| 1:b:74:TYR:HA   | 1:b:328:ALA:HB3 | 1.96                     | 0.47              |
| 1:A:383:ALA:HB1 | 2:E:290:GLU:HA  | 1.95                     | 0.47              |
| 1:B:152:HIS:HA  | 1:B:182:THR:HA  | 1.96                     | 0.47              |
| 1:b:61:VAL:HA   | 1:b:71:ILE:HA   | 1.98                     | 0.46              |
| 2:f:278:LEU:H   | 2:f:333:PRO:HA  | 1.81                     | 0.46              |
| 1:B:61:VAL:HA   | 1:B:71:ILE:HA   | 1.97                     | 0.45              |
| 1:a:61:VAL:HA   | 1:a:71:ILE:HA   | 1.99                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:61:VAL:HA   | 1:A:71:ILE:HA   | 1.99                     | 0.45              |
| 1:c:390:ALA:HB1 | 2:d:245:ALA:HB1 | 1.99                     | 0.45              |
| 2:F:278:LEU:H   | 2:F:333:PRO:HA  | 1.81                     | 0.45              |
| 1:C:493:ALA:HB1 | 1:C:519:ALA:HB2 | 1.99                     | 0.44              |
| 1:C:500:VAL:O   | 1:C:504:GLY:N   | 2.48                     | 0.44              |
| 1:c:29:TYR:O    | 2:f:72:GLY:N    | 2.39                     | 0.44              |
| 1:c:493:ALA:HB1 | 1:c:519:ALA:HB2 | 1.99                     | 0.44              |
| 2:e:28:TYR:N    | 2:e:93:VAL:O    | 2.52                     | 0.43              |
| 2:e:29:ASN:HA   | 2:e:92:THR:HA   | 1.99                     | 0.43              |
| 1:A:398:LYS:HA  | 1:A:410:SER:HA  | 2.01                     | 0.43              |
| 2:E:28:TYR:N    | 2:E:93:VAL:O    | 2.52                     | 0.43              |
| 2:E:29:ASN:HA   | 2:E:92:THR:HA   | 1.99                     | 0.43              |
| 2:e:140:ASN:O   | 2:e:144:ARG:N   | 2.52                     | 0.43              |
| 1:a:163:PHE:HA  | 1:a:170:SER:HA  | 2.01                     | 0.43              |
| 2:F:44:VAL:N    | 2:F:73:ASP:O    | 2.37                     | 0.43              |
| 1:c:233:PRO:HA  | 1:c:248:VAL:HA  | 2.01                     | 0.43              |
| 1:C:233:PRO:HA  | 1:C:248:VAL:HA  | 2.01                     | 0.42              |
| 1:a:64:ILE:HA   | 1:a:69:ALA:HA   | 2.02                     | 0.42              |
| 1:a:398:LYS:HA  | 1:a:410:SER:HA  | 2.01                     | 0.42              |
| 1:b:143:THR:HA  | 1:b:189:ALA:HB1 | 2.01                     | 0.42              |
| 2:E:140:ASN:O   | 2:E:144:ARG:N   | 2.52                     | 0.42              |
| 1:a:198:ILE:H   | 1:a:211:THR:HA  | 1.85                     | 0.42              |
| 1:B:162:VAL:O   | 1:B:171:HIS:N   | 2.40                     | 0.42              |
| 1:A:198:ILE:H   | 1:A:211:THR:HA  | 1.85                     | 0.41              |
| 2:D:214:ALA:HB3 | 2:D:242:LEU:HA  | 2.02                     | 0.41              |
| 2:F:67:VAL:HA   | 2:F:77:VAL:HA   | 2.02                     | 0.41              |
| 1:A:163:PHE:HA  | 1:A:170:SER:HA  | 2.01                     | 0.41              |
| 1:A:64:ILE:HA   | 1:A:69:ALA:HA   | 2.02                     | 0.41              |
| 2:E:173:PHE:O   | 2:E:360:VAL:N   | 2.49                     | 0.41              |
| 1:B:143:THR:HA  | 1:B:189:ALA:HB1 | 2.01                     | 0.41              |
| 2:d:167:GLY:HA2 | 2:d:320:GLY:HA2 | 2.03                     | 0.41              |
| 2:F:276:THR:O   | 2:F:332:ILE:N   | 2.36                     | 0.40              |
| 2:f:67:VAL:HA   | 2:f:77:VAL:HA   | 2.03                     | 0.40              |
| 2:f:276:THR:O   | 2:f:332:ILE:N   | 2.36                     | 0.40              |
| 1:c:500:VAL:O   | 1:c:504:GLY:N   | 2.48                     | 0.40              |

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     | 589/617 (96%) | 550 (93%)  | 34 (6%) | 5 (1%)   | 16          | 54  |
| 1   | B     | 592/617 (96%) | 557 (94%)  | 35 (6%) | 0        | 100         | 100 |
| 1   | C     | 587/617 (95%) | 548 (93%)  | 33 (6%) | 6 (1%)   | 12          | 48  |
| 1   | a     | 589/617 (96%) | 550 (93%)  | 33 (6%) | 6 (1%)   | 12          | 48  |
| 1   | b     | 587/617 (95%) | 552 (94%)  | 35 (6%) | 0        | 100         | 100 |
| 1   | c     | 584/617 (95%) | 545 (93%)  | 33 (6%) | 6 (1%)   | 12          | 48  |
| 2   | D     | 453/517 (88%) | 425 (94%)  | 28 (6%) | 0        | 100         | 100 |
| 2   | E     | 449/517 (87%) | 428 (95%)  | 21 (5%) | 0        | 100         | 100 |
| 2   | F     | 445/517 (86%) | 420 (94%)  | 25 (6%) | 0        | 100         | 100 |
| 2   | d     | 458/517 (89%) | 429 (94%)  | 28 (6%) | 1 (0%)   | 43          | 78  |
| 2   | e     | 452/517 (87%) | 431 (95%)  | 21 (5%) | 0        | 100         | 100 |
| 2   | f     | 445/517 (86%) | 421 (95%)  | 23 (5%) | 1 (0%)   | 43          | 78  |
| 3   | H     | 439/478 (92%) | 412 (94%)  | 27 (6%) | 0        | 100         | 100 |
| 3   | h     | 438/478 (92%) | 412 (94%)  | 25 (6%) | 1 (0%)   | 43          | 78  |
| 4   | G     | 135/256 (53%) | 130 (96%)  | 4 (3%)  | 1 (1%)   | 18          | 56  |
| 4   | g     | 137/256 (54%) | 134 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 5   | J     | 102/122 (84%) | 100 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 5   | L     | 66/122 (54%)  | 65 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 5   | N     | 79/122 (65%)  | 75 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 5   | j     | 99/122 (81%)  | 97 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 5   | l     | 64/122 (52%)  | 63 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 5   | n     | 54/122 (44%)  | 51 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 6   | I     | 214/233 (92%) | 213 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 6   | K     | 176/233 (76%) | 175 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 6   | M     | 201/233 (86%) | 200 (100%) | 1 (0%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 6   | i     | 215/233 (92%)    | 213 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 6   | k     | 166/233 (71%)    | 165 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 6   | m     | 179/233 (77%)    | 178 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| All | All   | 8994/10402 (86%) | 8539 (95%) | 428 (5%) | 27 (0%)  | 36          | 72  |

All (27) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 187 | ALA  |
| 1   | C     | 188 | PRO  |
| 4   | G     | 138 | ILE  |
| 1   | c     | 187 | ALA  |
| 1   | c     | 188 | PRO  |
| 1   | A     | 589 | GLU  |
| 1   | C     | 144 | PRO  |
| 1   | a     | 589 | GLU  |
| 1   | c     | 144 | PRO  |
| 1   | A     | 590 | PRO  |
| 1   | C     | 305 | MET  |
| 3   | h     | 152 | GLN  |
| 1   | a     | 590 | PRO  |
| 1   | c     | 305 | MET  |
| 2   | d     | 200 | VAL  |
| 1   | A     | 187 | ALA  |
| 1   | A     | 309 | LYS  |
| 1   | A     | 476 | TYR  |
| 1   | a     | 187 | ALA  |
| 1   | a     | 309 | LYS  |
| 1   | C     | 145 | GLY  |
| 1   | C     | 146 | LYS  |
| 1   | c     | 145 | GLY  |
| 1   | c     | 146 | LYS  |
| 1   | a     | 477 | PRO  |
| 1   | a     | 452 | PHE  |
| 2   | f     | 370 | TYR  |

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 oligosaccharides 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> ) | Q < 0.9 |
|-----|-------|---------------|--------|-----------|-----|-----|-----------------------|---------|
| 1   | A     | 591/617 (95%) | -0.01  | 17 (2%)   | 53  | 47  | 126, 311, 475, 652    | 0       |
| 1   | B     | 594/617 (96%) | -0.14  | 14 (2%)   | 59  | 52  | 107, 290, 447, 594    | 0       |
| 1   | C     | 589/617 (95%) | 0.00   | 19 (3%)   | 50  | 45  | 111, 281, 475, 610    | 0       |
| 1   | a     | 591/617 (95%) | 0.15   | 28 (4%)   | 36  | 37  | 126, 314, 475, 658    | 0       |
| 1   | b     | 589/617 (95%) | -0.12  | 9 (1%)    | 72  | 60  | 107, 292, 450, 597    | 0       |
| 1   | c     | 586/617 (94%) | -0.05  | 15 (2%)   | 57  | 49  | 111, 282, 473, 614    | 0       |
| 2   | D     | 457/517 (88%) | 0.01   | 13 (2%)   | 55  | 48  | 92, 239, 384, 587     | 0       |
| 2   | E     | 453/517 (87%) | 0.10   | 11 (2%)   | 59  | 52  | 124, 258, 413, 663    | 0       |
| 2   | F     | 449/517 (86%) | -0.03  | 10 (2%)   | 62  | 53  | 146, 287, 414, 584    | 0       |
| 2   | d     | 460/517 (88%) | -0.09  | 10 (2%)   | 62  | 53  | 94, 241, 390, 586     | 0       |
| 2   | e     | 456/517 (88%) | -0.01  | 13 (2%)   | 53  | 47  | 125, 258, 415, 667    | 0       |
| 2   | f     | 449/517 (86%) | -0.05  | 10 (2%)   | 62  | 53  | 145, 288, 416, 573    | 0       |
| 3   | H     | 445/478 (93%) | -0.31  | 4 (0%)    | 81  | 70  | 65, 163, 317, 625     | 0       |
| 3   | h     | 444/478 (92%) | -0.22  | 7 (1%)    | 70  | 59  | 61, 164, 321, 631     | 0       |
| 4   | G     | 139/256 (54%) | -0.28  | 2 (1%)    | 73  | 62  | 93, 212, 488, 554     | 0       |
| 4   | g     | 141/256 (55%) | -0.32  | 1 (0%)    | 84  | 74  | 97, 213, 493, 560     | 0       |
| 5   | J     | 104/122 (85%) | -0.20  | 2 (1%)    | 66  | 56  | 154, 290, 427, 498    | 0       |
| 5   | L     | 68/122 (55%)  | 0.22   | 3 (4%)    | 39  | 39  | 283, 418, 525, 566    | 0       |
| 5   | N     | 81/122 (66%)  | -0.10  | 2 (2%)    | 58  | 50  | 200, 450, 574, 740    | 0       |
| 5   | j     | 101/122 (82%) | -0.31  | 0         | 100 | 100 | 151, 282, 419, 497    | 0       |
| 5   | l     | 66/122 (54%)  | -0.14  | 0         | 100 | 100 | 279, 422, 522, 566    | 0       |
| 5   | n     | 58/122 (47%)  | -0.13  | 2 (3%)    | 48  | 44  | 200, 441, 509, 541    | 0       |
| 6   | I     | 216/233 (92%) | 0.17   | 13 (6%)   | 27  | 32  | 112, 345, 497, 643    | 0       |
| 6   | K     | 178/233 (76%) | -0.13  | 4 (2%)    | 62  | 53  | 186, 344, 491, 599    | 0       |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------|----|----|-----------------------|-------|
| 6   | M     | 203/233 (87%)    | 0.13   | 6 (2%)   | 52 | 46 | 200, 410, 571, 626    | 0     |
| 6   | i     | 217/233 (93%)    | 0.02   | 8 (3%)   | 45 | 43 | 91, 345, 511, 638     | 0     |
| 6   | k     | 168/233 (72%)    | 0.22   | 6 (3%)   | 46 | 43 | 187, 331, 466, 514    | 0     |
| 6   | m     | 181/233 (77%)    | 0.03   | 5 (2%)   | 55 | 48 | 200, 402, 542, 587    | 0     |
| All | All   | 9074/10402 (87%) | -0.05  | 234 (2%) | 57 | 49 | 61, 281, 479, 740     | 0     |

All (234) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 123 | ILE  | 7.4  |
| 2   | e     | 105 | SER  | 5.3  |
| 1   | B     | 123 | ILE  | 5.3  |
| 3   | h     | 473 | ILE  | 5.2  |
| 1   | A     | 151 | ASP  | 5.0  |
| 3   | H     | 134 | GLY  | 5.0  |
| 1   | B     | 468 | LEU  | 4.7  |
| 3   | h     | 476 | THR  | 4.7  |
| 2   | F     | 87  | ASP  | 4.6  |
| 6   | I     | 117 | TYR  | 4.6  |
| 1   | A     | 541 | ILE  | 4.5  |
| 3   | H     | 385 | ASP  | 4.5  |
| 2   | d     | 156 | SER  | 4.4  |
| 2   | e     | 262 | THR  | 4.4  |
| 6   | I     | 48  | THR  | 4.2  |
| 6   | k     | 137 | ALA  | 4.2  |
| 1   | C     | 465 | THR  | 4.1  |
| 6   | m     | 187 | GLY  | 4.0  |
| 6   | I     | 187 | GLY  | 3.9  |
| 1   | A     | 462 | SER  | 3.9  |
| 1   | c     | 179 | SER  | 3.9  |
| 1   | C     | 532 | TYR  | 3.9  |
| 1   | a     | 198 | ILE  | 3.9  |
| 1   | C     | 467 | VAL  | 3.9  |
| 1   | b     | 421 | GLY  | 3.8  |
| 2   | D     | 326 | ASN  | 3.8  |
| 2   | d     | 399 | VAL  | 3.8  |
| 1   | a     | 347 | GLN  | 3.8  |
| 1   | a     | 304 | GLU  | 3.8  |
| 2   | f     | 230 | GLU  | 3.8  |
| 6   | i     | 187 | GLY  | 3.7  |
| 5   | L     | 65  | VAL  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 577 | ASP  | 3.7  |
| 2   | d     | 203 | GLY  | 3.7  |
| 3   | h     | 475 | TYR  | 3.7  |
| 1   | C     | 512 | ASP  | 3.7  |
| 1   | C     | 42  | ILE  | 3.6  |
| 2   | D     | 318 | ARG  | 3.6  |
| 1   | C     | 386 | GLY  | 3.6  |
| 6   | I     | 223 | TYR  | 3.6  |
| 1   | b     | 420 | ALA  | 3.4  |
| 1   | b     | 247 | CYS  | 3.4  |
| 2   | F     | 86  | ILE  | 3.4  |
| 5   | J     | 103 | ILE  | 3.4  |
| 1   | A     | 148 | GLN  | 3.4  |
| 1   | a     | 192 | TYR  | 3.4  |
| 1   | A     | 463 | LYS  | 3.3  |
| 1   | c     | 571 | LEU  | 3.3  |
| 6   | i     | 48  | THR  | 3.3  |
| 1   | a     | 462 | SER  | 3.3  |
| 6   | i     | 62  | PHE  | 3.3  |
| 6   | I     | 31  | LYS  | 3.3  |
| 2   | F     | 88  | VAL  | 3.3  |
| 2   | e     | 106 | GLU  | 3.3  |
| 6   | I     | 121 | LEU  | 3.3  |
| 1   | a     | 541 | ILE  | 3.3  |
| 1   | b     | 99  | PRO  | 3.2  |
| 1   | B     | 288 | GLY  | 3.2  |
| 2   | E     | 343 | THR  | 3.2  |
| 6   | M     | 187 | GLY  | 3.2  |
| 5   | N     | 94  | VAL  | 3.2  |
| 1   | B     | 99  | PRO  | 3.2  |
| 2   | D     | 177 | GLY  | 3.2  |
| 2   | D     | 198 | LYS  | 3.1  |
| 2   | E     | 424 | ALA  | 3.2  |
| 1   | a     | 88  | ARG  | 3.1  |
| 2   | E     | 104 | VAL  | 3.1  |
| 6   | k     | 187 | GLY  | 3.1  |
| 6   | I     | 120 | ILE  | 3.1  |
| 1   | a     | 391 | SER  | 3.1  |
| 2   | f     | 399 | VAL  | 3.1  |
| 1   | A     | 27  | ALA  | 3.1  |
| 2   | f     | 402 | GLN  | 3.1  |
| 1   | B     | 421 | GLY  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | f     | 187 | ILE  | 3.1  |
| 6   | k     | 185 | SER  | 3.0  |
| 2   | E     | 176 | SER  | 3.0  |
| 1   | a     | 99  | PRO  | 3.0  |
| 2   | f     | 128 | ALA  | 3.0  |
| 1   | B     | 168 | ILE  | 3.0  |
| 1   | a     | 585 | SER  | 2.9  |
| 1   | A     | 550 | ALA  | 2.9  |
| 1   | b     | 85  | PRO  | 2.9  |
| 1   | c     | 377 | ALA  | 2.9  |
| 3   | H     | 10  | SER  | 2.9  |
| 6   | M     | 99  | ILE  | 2.8  |
| 6   | m     | 62  | PHE  | 2.8  |
| 1   | C     | 574 | SER  | 2.8  |
| 2   | E     | 268 | TYR  | 2.8  |
| 2   | d     | 472 | MET  | 2.8  |
| 6   | k     | 122 | GLN  | 2.8  |
| 2   | D     | 299 | PRO  | 2.8  |
| 1   | a     | 586 | LYS  | 2.7  |
| 6   | i     | 54  | GLU  | 2.7  |
| 2   | E     | 349 | LEU  | 2.7  |
| 1   | b     | 550 | ALA  | 2.7  |
| 1   | C     | 355 | ALA  | 2.7  |
| 2   | f     | 87  | ASP  | 2.7  |
| 1   | b     | 320 | ALA  | 2.7  |
| 2   | D     | 239 | SER  | 2.7  |
| 1   | a     | 362 | ALA  | 2.7  |
| 2   | D     | 294 | ALA  | 2.7  |
| 1   | A     | 379 | GLN  | 2.6  |
| 1   | B     | 96  | GLU  | 2.6  |
| 1   | b     | 235 | LEU  | 2.6  |
| 1   | A     | 399 | ALA  | 2.6  |
| 1   | B     | 166 | SER  | 2.6  |
| 2   | d     | 141 | PRO  | 2.6  |
| 2   | d     | 459 | ASP  | 2.6  |
| 1   | a     | 320 | ALA  | 2.6  |
| 5   | n     | 87  | ALA  | 2.6  |
| 6   | k     | 128 | ALA  | 2.6  |
| 6   | M     | 223 | TYR  | 2.6  |
| 1   | C     | 135 | ASP  | 2.6  |
| 2   | D     | 395 | ASP  | 2.5  |
| 1   | a     | 52  | VAL  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 246 | ASN  | 2.5  |
| 1   | A     | 99  | PRO  | 2.5  |
| 1   | a     | 123 | ILE  | 2.5  |
| 2   | F     | 83  | THR  | 2.5  |
| 2   | D     | 478 | PRO  | 2.5  |
| 1   | C     | 469 | ASN  | 2.5  |
| 2   | E     | 342 | ILE  | 2.5  |
| 6   | I     | 20  | MET  | 2.5  |
| 1   | a     | 323 | SER  | 2.5  |
| 1   | c     | 233 | PRO  | 2.5  |
| 1   | A     | 150 | GLY  | 2.5  |
| 2   | e     | 264 | GLU  | 2.5  |
| 6   | I     | 186 | GLY  | 2.5  |
| 1   | c     | 561 | ALA  | 2.5  |
| 2   | f     | 336 | THR  | 2.4  |
| 1   | C     | 384 | TYR  | 2.4  |
| 6   | m     | 80  | ILE  | 2.4  |
| 1   | C     | 122 | SER  | 2.4  |
| 6   | K     | 149 | ILE  | 2.4  |
| 2   | D     | 156 | SER  | 2.4  |
| 2   | d     | 294 | ALA  | 2.4  |
| 2   | d     | 395 | ASP  | 2.4  |
| 3   | h     | 301 | ARG  | 2.4  |
| 1   | C     | 179 | SER  | 2.4  |
| 2   | F     | 349 | LEU  | 2.4  |
| 2   | F     | 421 | GLY  | 2.4  |
| 1   | A     | 526 | PHE  | 2.4  |
| 1   | a     | 584 | SER  | 2.4  |
| 1   | B     | 260 | GLY  | 2.3  |
| 5   | J     | 43  | ILE  | 2.3  |
| 6   | M     | 35  | ILE  | 2.3  |
| 6   | M     | 200 | ASN  | 2.3  |
| 6   | I     | 129 | LEU  | 2.3  |
| 3   | h     | 297 | CYS  | 2.3  |
| 1   | a     | 409 | GLY  | 2.3  |
| 2   | e     | 246 | ASN  | 2.3  |
| 1   | C     | 408 | THR  | 2.3  |
| 6   | m     | 199 | ILE  | 2.3  |
| 3   | H     | 475 | TYR  | 2.3  |
| 2   | D     | 163 | SER  | 2.3  |
| 2   | F     | 461 | ALA  | 2.3  |
| 6   | k     | 126 | VAL  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | L     | 44  | ASP  | 2.3  |
| 1   | a     | 146 | LYS  | 2.2  |
| 1   | b     | 340 | LEU  | 2.2  |
| 6   | I     | 214 | ALA  | 2.2  |
| 6   | K     | 66  | LEU  | 2.2  |
| 4   | G     | 175 | HIS  | 2.2  |
| 1   | a     | 336 | THR  | 2.2  |
| 1   | a     | 86  | VAL  | 2.2  |
| 5   | N     | 65  | VAL  | 2.2  |
| 6   | i     | 120 | ILE  | 2.2  |
| 6   | m     | 75  | ILE  | 2.2  |
| 6   | i     | 96  | LEU  | 2.2  |
| 1   | A     | 387 | ALA  | 2.2  |
| 1   | B     | 465 | THR  | 2.2  |
| 1   | A     | 509 | SER  | 2.2  |
| 1   | C     | 317 | THR  | 2.2  |
| 2   | e     | 130 | ASP  | 2.2  |
| 1   | c     | 33  | GLY  | 2.2  |
| 2   | E     | 324 | GLY  | 2.2  |
| 3   | h     | 474 | GLY  | 2.2  |
| 1   | a     | 511 | SER  | 2.2  |
| 4   | g     | 175 | HIS  | 2.2  |
| 1   | B     | 231 | ASP  | 2.2  |
| 2   | d     | 202 | ASP  | 2.2  |
| 1   | C     | 66  | GLY  | 2.2  |
| 2   | d     | 157 | ALA  | 2.2  |
| 2   | e     | 410 | GLY  | 2.2  |
| 2   | f     | 214 | ALA  | 2.2  |
| 2   | e     | 50  | ASN  | 2.2  |
| 2   | F     | 127 | PHE  | 2.2  |
| 2   | F     | 234 | SER  | 2.2  |
| 1   | c     | 247 | CYS  | 2.2  |
| 6   | K     | 145 | ASP  | 2.1  |
| 1   | A     | 386 | GLY  | 2.1  |
| 1   | c     | 380 | GLY  | 2.1  |
| 2   | f     | 395 | ASP  | 2.1  |
| 1   | B     | 354 | ILE  | 2.1  |
| 1   | c     | 244 | LEU  | 2.1  |
| 2   | e     | 403 | LEU  | 2.1  |
| 2   | e     | 135 | ASN  | 2.1  |
| 1   | a     | 239 | ARG  | 2.1  |
| 2   | F     | 402 | GLN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 566 | ALA  | 2.1  |
| 1   | c     | 153 | ILE  | 2.1  |
| 2   | D     | 107 | ASP  | 2.1  |
| 1   | A     | 591 | SER  | 2.1  |
| 1   | c     | 32  | SER  | 2.1  |
| 2   | D     | 320 | GLY  | 2.1  |
| 2   | f     | 465 | LEU  | 2.1  |
| 6   | I     | 19  | LYS  | 2.1  |
| 6   | i     | 45  | ILE  | 2.1  |
| 1   | c     | 554 | TYR  | 2.1  |
| 1   | C     | 531 | GLY  | 2.1  |
| 5   | L     | 90  | LYS  | 2.1  |
| 1   | A     | 512 | ASP  | 2.1  |
| 1   | a     | 512 | ASP  | 2.1  |
| 2   | e     | 35  | ASN  | 2.1  |
| 1   | c     | 183 | ILE  | 2.1  |
| 2   | e     | 323 | GLU  | 2.1  |
| 6   | i     | 33  | LYS  | 2.1  |
| 1   | C     | 575 | THR  | 2.1  |
| 5   | n     | 94  | VAL  | 2.1  |
| 6   | I     | 51  | VAL  | 2.1  |
| 6   | M     | 172 | ILE  | 2.0  |
| 1   | a     | 513 | LYS  | 2.0  |
| 1   | c     | 386 | GLY  | 2.0  |
| 2   | E     | 192 | GLY  | 2.0  |
| 6   | K     | 187 | GLY  | 2.0  |
| 1   | c     | 457 | THR  | 2.0  |
| 1   | B     | 100 | GLY  | 2.0  |
| 3   | h     | 378 | GLY  | 2.0  |
| 2   | E     | 347 | PRO  | 2.0  |
| 4   | G     | 147 | VAL  | 2.0  |
| 1   | B     | 289 | ASN  | 2.0  |
| 1   | a     | 394 | GLU  | 2.0  |
| 2   | e     | 166 | ARG  | 2.0  |

## 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 [i](#)

There are no oligosaccharides 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.