



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 01:53 am GMT

PDB ID : 9G3O  
EMDB ID : EMD-51005  
Title : Circularly permuted lumazine synthase 24-pentamer spherical cage  
Authors : Koziej, L.; Azuma, Y.  
Deposited on : 2024-07-12  
Resolution : 2.76 Å(reported)  
Based on initial model : 1HQK

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

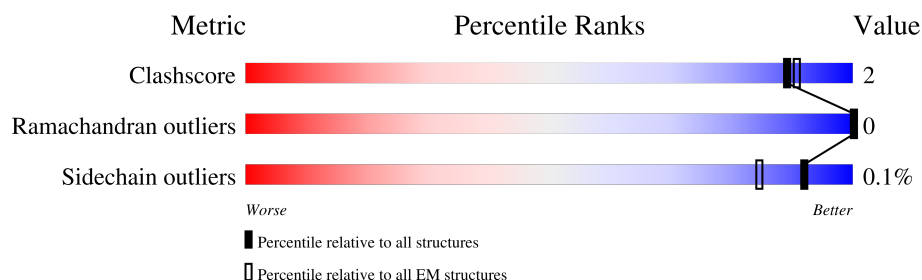
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.76 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) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 163    | 88% . 9%         |
| 1   | AA    | 163    | 90% . 9%         |
| 1   | AB    | 163    | 87% . 9%         |
| 1   | AC    | 163    | 89% . 9%         |
| 1   | AD    | 163    | 88% 5% 7%        |
| 1   | B     | 163    | 88% . 9%         |
| 1   | BA    | 163    | 90% . 6%         |
| 1   | BB    | 163    | 85% 5% 10%       |
| 1   | BC    | 163    | 88% . 8%         |


























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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | BD    | 163    |    |
| 1   | C     | 163    |    |
| 1   | CA    | 163    |    |
| 1   | CB    | 163    |    |
| 1   | CC    | 163    |    |
| 1   | CD    | 163    |    |
| 1   | D     | 163    |    |
| 1   | DA    | 163    |    |
| 1   | DB    | 163    |    |
| 1   | DC    | 163    |    |
| 1   | DD    | 163    |    |
| 1   | E     | 163    |   |
| 1   | EA    | 163    |  |
| 1   | EB    | 163    |  |
| 1   | EC    | 163    |  |
| 1   | ED    | 163    |  |
| 1   | F     | 163    |  |
| 1   | FA    | 163    |  |
| 1   | FB    | 163    |  |
| 1   | FC    | 163    |  |
| 1   | FD    | 163    |  |
| 1   | G     | 163    |  |
| 1   | GA    | 163    |  |
| 1   | GB    | 163    |  |
| 1   | GC    | 163    |  |


























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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | GD    | 163    |    |
| 1   | H     | 163    |    |
| 1   | HA    | 163    |    |
| 1   | HB    | 163    |    |
| 1   | HC    | 163    |    |
| 1   | HD    | 163    |    |
| 1   | I     | 163    |    |
| 1   | IA    | 163    |    |
| 1   | IB    | 163    |    |
| 1   | IC    | 163    |    |
| 1   | ID    | 163    |    |
| 1   | J     | 163    |   |
| 1   | JA    | 163    |  |
| 1   | JB    | 163    |  |
| 1   | JC    | 163    |  |
| 1   | JD    | 163    |  |
| 1   | K     | 163    |  |
| 1   | KA    | 163    |  |
| 1   | KB    | 163    |  |
| 1   | KC    | 163    |  |
| 1   | KD    | 163    |  |
| 1   | L     | 163    |  |
| 1   | LA    | 163    |  |
| 1   | LB    | 163    |  |
| 1   | LC    | 163    |  |












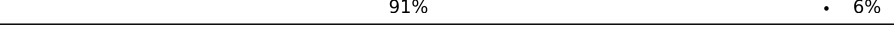







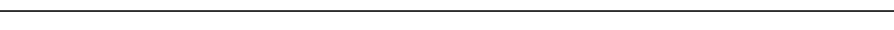

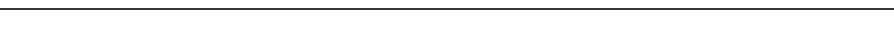
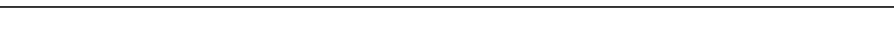


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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | LD    | 163    |    |
| 1   | M     | 163    |    |
| 1   | MA    | 163    |    |
| 1   | MB    | 163    |    |
| 1   | MC    | 163    |    |
| 1   | MD    | 163    |    |
| 1   | N     | 163    |    |
| 1   | NA    | 163    |    |
| 1   | NB    | 163    |    |
| 1   | NC    | 163    |    |
| 1   | ND    | 163    |    |
| 1   | O     | 163    |   |
| 1   | OA    | 163    |  |
| 1   | OB    | 163    |  |
| 1   | OC    | 163    |  |
| 1   | OD    | 163    |  |
| 1   | P     | 163    |  |
| 1   | PA    | 163    |  |
| 1   | PB    | 163    |  |
| 1   | PC    | 163    |  |
| 1   | PD    | 163    |  |
| 1   | Q     | 163    |  |
| 1   | QA    | 163    |  |
| 1   | QB    | 163    |  |
| 1   | QC    | 163    |  |


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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | R     | 163    |  90% • 6%     |
| 1   | RA    | 163    |  85% 5% 10%   |
| 1   | RB    | 163    |  88% • 8%     |
| 1   | RC    | 163    |  83% 7% 10%   |
| 1   | S     | 163    |  89% • 9%     |
| 1   | SA    | 163    |  88% 5% 7%    |
| 1   | SB    | 163    |  88% • 9%     |
| 1   | SC    | 163    |  90% • 9%     |
| 1   | T     | 163    |  89% • 8%     |
| 1   | TA    | 163    |  83% 7% 10%   |
| 1   | TB    | 163    |  89% • 9%     |
| 1   | TC    | 163    |  91% • 6%    |
| 1   | U     | 163    |  88% • 9%   |
| 1   | UA    | 163    |  89% • 9%   |
| 1   | UB    | 163    |  87% • 9%   |
| 1   | UC    | 163    |  89% • 9%   |
| 1   | V     | 163    |  89% • 9%   |
| 1   | VA    | 163    |  90% • 6%   |
| 1   | VB    | 163    |  85% 5% 10% |
| 1   | VC    | 163    |  88% • 8%   |
| 1   | W     | 163    |  87% • 9%   |
| 1   | WA    | 163    |  89% • 9%   |
| 1   | WB    | 163    |  88% 5% 7%  |
| 1   | WC    | 163    |  88% • 9%   |
| 1   | X     | 163    |  86% • 10%  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | XA    | 163    |  89% 8%     |
| 1   | XB    | 163    |  83% 7% 10% |
| 1   | XC    | 163    |  88% 9%     |
| 1   | Y     | 163    |  88% 5% 7%  |
| 1   | YA    | 163    |  88% 9%     |
| 1   | YB    | 163    |  90% 9%     |
| 1   | YC    | 163    |  87% 9%     |
| 1   | Z     | 163    |  83% 7% 10% |
| 1   | ZA    | 163    |  89% 9%     |
| 1   | ZB    | 163    |  90% 6%     |
| 1   | ZC    | 163    |  86% 10%    |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 133824 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 6,7-dimethyl-8-ribityllumazine synthase.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | B     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | C     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | D     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | E     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | F     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | G     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | H     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | I     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | J     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | K     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | L     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | M     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | N     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | O     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | P     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | Q     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | R     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | S     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | T     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | U     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | V     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | W     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | X     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | Y     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | Z     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | AA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | BA    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | CA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | DA    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | EA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | FA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | GA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | HA    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | IA    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | JA    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | KA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | LA    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | MA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | NA    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | OA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | PA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | QA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | RA    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | SA    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | TA    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | UA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | VA    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | WA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | XA    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | YA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | ZA    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | AB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | BB    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | CB    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | DB    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | EB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | FB    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | GB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | HB    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | IB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | JB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | KB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | LB    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | MB    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | NB    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | OB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | PB    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | QB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | RB    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | SB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | TB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | UB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | VB    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | WB    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | XB    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | YB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | ZB    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | AC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | BC    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | CC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | DC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | EC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | FC    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | GC    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | HC    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | IC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | JC    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | KC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | LC    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | MC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | NC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | OC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | PC    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | QC    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | RC    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | SC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | TC    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | UC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | VC    | 150      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | WC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | XC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | YC    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | ZC    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | AD    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | BD    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | CD    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | DD    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | ED    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | FD    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |
| 1   | GD    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | HD    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | ID    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | JD    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | KD    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 202 | 212 | 3 |         |       |
| 1   | LD    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 699 | 195 | 207 | 3 |         |       |
| 1   | MD    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | ND    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 722 | 204 | 214 | 3 |         |       |
| 1   | OD    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 196 | 208 | 3 |         |       |
| 1   | PD    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 713 | 201 | 210 | 3 |         |       |

There are 1320 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | MET      | -      | initiating methionine | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 37      | GLY      | -      | linker                | UNP O66529 |
| A     | 38      | THR      | -      | linker                | UNP O66529 |
| A     | 39      | GLY      | -      | linker                | UNP O66529 |
| A     | 40      | GLY      | -      | linker                | UNP O66529 |
| A     | 41      | SER      | -      | linker                | UNP O66529 |
| A     | 42      | GLY      | -      | linker                | UNP O66529 |
| A     | 43      | SER      | -      | linker                | UNP O66529 |
| A     | 44      | SER      | -      | linker                | UNP O66529 |
| A     | 45      | MET      | -      | linker                | UNP O66529 |
| A     | 46      | GLU      | -      | linker                | UNP O66529 |
| B     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| B     | 37      | GLY      | -      | linker                | UNP O66529 |
| B     | 38      | THR      | -      | linker                | UNP O66529 |
| B     | 39      | GLY      | -      | linker                | UNP O66529 |
| B     | 40      | GLY      | -      | linker                | UNP O66529 |
| B     | 41      | SER      | -      | linker                | UNP O66529 |
| B     | 42      | GLY      | -      | linker                | UNP O66529 |
| B     | 43      | SER      | -      | linker                | UNP O66529 |
| B     | 44      | SER      | -      | linker                | UNP O66529 |
| B     | 45      | MET      | -      | linker                | UNP O66529 |
| B     | 46      | GLU      | -      | linker                | UNP O66529 |
| C     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| C     | 37      | GLY      | -      | linker                | UNP O66529 |
| C     | 38      | THR      | -      | linker                | UNP O66529 |
| C     | 39      | GLY      | -      | linker                | UNP O66529 |
| C     | 40      | GLY      | -      | linker                | UNP O66529 |
| C     | 41      | SER      | -      | linker                | UNP O66529 |
| C     | 42      | GLY      | -      | linker                | UNP O66529 |
| C     | 43      | SER      | -      | linker                | UNP O66529 |
| C     | 44      | SER      | -      | linker                | UNP O66529 |
| C     | 45      | MET      | -      | linker                | UNP O66529 |
| C     | 46      | GLU      | -      | linker                | UNP O66529 |
| D     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| D     | 37      | GLY      | -      | linker                | UNP O66529 |
| D     | 38      | THR      | -      | linker                | UNP O66529 |
| D     | 39      | GLY      | -      | linker                | UNP O66529 |
| D     | 40      | GLY      | -      | linker                | UNP O66529 |
| D     | 41      | SER      | -      | linker                | UNP O66529 |
| D     | 42      | GLY      | -      | linker                | UNP O66529 |
| D     | 43      | SER      | -      | linker                | UNP O66529 |
| D     | 44      | SER      | -      | linker                | UNP O66529 |
| D     | 45      | MET      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| D     | 46      | GLU      | -      | linker                | UNP O66529 |
| E     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| E     | 37      | GLY      | -      | linker                | UNP O66529 |
| E     | 38      | THR      | -      | linker                | UNP O66529 |
| E     | 39      | GLY      | -      | linker                | UNP O66529 |
| E     | 40      | GLY      | -      | linker                | UNP O66529 |
| E     | 41      | SER      | -      | linker                | UNP O66529 |
| E     | 42      | GLY      | -      | linker                | UNP O66529 |
| E     | 43      | SER      | -      | linker                | UNP O66529 |
| E     | 44      | SER      | -      | linker                | UNP O66529 |
| E     | 45      | MET      | -      | linker                | UNP O66529 |
| E     | 46      | GLU      | -      | linker                | UNP O66529 |
| F     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| F     | 37      | GLY      | -      | linker                | UNP O66529 |
| F     | 38      | THR      | -      | linker                | UNP O66529 |
| F     | 39      | GLY      | -      | linker                | UNP O66529 |
| F     | 40      | GLY      | -      | linker                | UNP O66529 |
| F     | 41      | SER      | -      | linker                | UNP O66529 |
| F     | 42      | GLY      | -      | linker                | UNP O66529 |
| F     | 43      | SER      | -      | linker                | UNP O66529 |
| F     | 44      | SER      | -      | linker                | UNP O66529 |
| F     | 45      | MET      | -      | linker                | UNP O66529 |
| F     | 46      | GLU      | -      | linker                | UNP O66529 |
| G     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| G     | 37      | GLY      | -      | linker                | UNP O66529 |
| G     | 38      | THR      | -      | linker                | UNP O66529 |
| G     | 39      | GLY      | -      | linker                | UNP O66529 |
| G     | 40      | GLY      | -      | linker                | UNP O66529 |
| G     | 41      | SER      | -      | linker                | UNP O66529 |
| G     | 42      | GLY      | -      | linker                | UNP O66529 |
| G     | 43      | SER      | -      | linker                | UNP O66529 |
| G     | 44      | SER      | -      | linker                | UNP O66529 |
| G     | 45      | MET      | -      | linker                | UNP O66529 |
| G     | 46      | GLU      | -      | linker                | UNP O66529 |
| H     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| H     | 37      | GLY      | -      | linker                | UNP O66529 |
| H     | 38      | THR      | -      | linker                | UNP O66529 |
| H     | 39      | GLY      | -      | linker                | UNP O66529 |
| H     | 40      | GLY      | -      | linker                | UNP O66529 |
| H     | 41      | SER      | -      | linker                | UNP O66529 |
| H     | 42      | GLY      | -      | linker                | UNP O66529 |
| H     | 43      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| H     | 44      | SER      | -      | linker                | UNP O66529 |
| H     | 45      | MET      | -      | linker                | UNP O66529 |
| H     | 46      | GLU      | -      | linker                | UNP O66529 |
| I     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| I     | 37      | GLY      | -      | linker                | UNP O66529 |
| I     | 38      | THR      | -      | linker                | UNP O66529 |
| I     | 39      | GLY      | -      | linker                | UNP O66529 |
| I     | 40      | GLY      | -      | linker                | UNP O66529 |
| I     | 41      | SER      | -      | linker                | UNP O66529 |
| I     | 42      | GLY      | -      | linker                | UNP O66529 |
| I     | 43      | SER      | -      | linker                | UNP O66529 |
| I     | 44      | SER      | -      | linker                | UNP O66529 |
| I     | 45      | MET      | -      | linker                | UNP O66529 |
| I     | 46      | GLU      | -      | linker                | UNP O66529 |
| J     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| J     | 37      | GLY      | -      | linker                | UNP O66529 |
| J     | 38      | THR      | -      | linker                | UNP O66529 |
| J     | 39      | GLY      | -      | linker                | UNP O66529 |
| J     | 40      | GLY      | -      | linker                | UNP O66529 |
| J     | 41      | SER      | -      | linker                | UNP O66529 |
| J     | 42      | GLY      | -      | linker                | UNP O66529 |
| J     | 43      | SER      | -      | linker                | UNP O66529 |
| J     | 44      | SER      | -      | linker                | UNP O66529 |
| J     | 45      | MET      | -      | linker                | UNP O66529 |
| J     | 46      | GLU      | -      | linker                | UNP O66529 |
| K     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| K     | 37      | GLY      | -      | linker                | UNP O66529 |
| K     | 38      | THR      | -      | linker                | UNP O66529 |
| K     | 39      | GLY      | -      | linker                | UNP O66529 |
| K     | 40      | GLY      | -      | linker                | UNP O66529 |
| K     | 41      | SER      | -      | linker                | UNP O66529 |
| K     | 42      | GLY      | -      | linker                | UNP O66529 |
| K     | 43      | SER      | -      | linker                | UNP O66529 |
| K     | 44      | SER      | -      | linker                | UNP O66529 |
| K     | 45      | MET      | -      | linker                | UNP O66529 |
| K     | 46      | GLU      | -      | linker                | UNP O66529 |
| L     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| L     | 37      | GLY      | -      | linker                | UNP O66529 |
| L     | 38      | THR      | -      | linker                | UNP O66529 |
| L     | 39      | GLY      | -      | linker                | UNP O66529 |
| L     | 40      | GLY      | -      | linker                | UNP O66529 |
| L     | 41      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| L     | 42      | GLY      | -      | linker                | UNP O66529 |
| L     | 43      | SER      | -      | linker                | UNP O66529 |
| L     | 44      | SER      | -      | linker                | UNP O66529 |
| L     | 45      | MET      | -      | linker                | UNP O66529 |
| L     | 46      | GLU      | -      | linker                | UNP O66529 |
| M     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| M     | 37      | GLY      | -      | linker                | UNP O66529 |
| M     | 38      | THR      | -      | linker                | UNP O66529 |
| M     | 39      | GLY      | -      | linker                | UNP O66529 |
| M     | 40      | GLY      | -      | linker                | UNP O66529 |
| M     | 41      | SER      | -      | linker                | UNP O66529 |
| M     | 42      | GLY      | -      | linker                | UNP O66529 |
| M     | 43      | SER      | -      | linker                | UNP O66529 |
| M     | 44      | SER      | -      | linker                | UNP O66529 |
| M     | 45      | MET      | -      | linker                | UNP O66529 |
| M     | 46      | GLU      | -      | linker                | UNP O66529 |
| N     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| N     | 37      | GLY      | -      | linker                | UNP O66529 |
| N     | 38      | THR      | -      | linker                | UNP O66529 |
| N     | 39      | GLY      | -      | linker                | UNP O66529 |
| N     | 40      | GLY      | -      | linker                | UNP O66529 |
| N     | 41      | SER      | -      | linker                | UNP O66529 |
| N     | 42      | GLY      | -      | linker                | UNP O66529 |
| N     | 43      | SER      | -      | linker                | UNP O66529 |
| N     | 44      | SER      | -      | linker                | UNP O66529 |
| N     | 45      | MET      | -      | linker                | UNP O66529 |
| N     | 46      | GLU      | -      | linker                | UNP O66529 |
| O     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| O     | 37      | GLY      | -      | linker                | UNP O66529 |
| O     | 38      | THR      | -      | linker                | UNP O66529 |
| O     | 39      | GLY      | -      | linker                | UNP O66529 |
| O     | 40      | GLY      | -      | linker                | UNP O66529 |
| O     | 41      | SER      | -      | linker                | UNP O66529 |
| O     | 42      | GLY      | -      | linker                | UNP O66529 |
| O     | 43      | SER      | -      | linker                | UNP O66529 |
| O     | 44      | SER      | -      | linker                | UNP O66529 |
| O     | 45      | MET      | -      | linker                | UNP O66529 |
| O     | 46      | GLU      | -      | linker                | UNP O66529 |
| P     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| P     | 37      | GLY      | -      | linker                | UNP O66529 |
| P     | 38      | THR      | -      | linker                | UNP O66529 |
| P     | 39      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| P     | 40      | GLY      | -      | linker                | UNP O66529 |
| P     | 41      | SER      | -      | linker                | UNP O66529 |
| P     | 42      | GLY      | -      | linker                | UNP O66529 |
| P     | 43      | SER      | -      | linker                | UNP O66529 |
| P     | 44      | SER      | -      | linker                | UNP O66529 |
| P     | 45      | MET      | -      | linker                | UNP O66529 |
| P     | 46      | GLU      | -      | linker                | UNP O66529 |
| Q     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| Q     | 37      | GLY      | -      | linker                | UNP O66529 |
| Q     | 38      | THR      | -      | linker                | UNP O66529 |
| Q     | 39      | GLY      | -      | linker                | UNP O66529 |
| Q     | 40      | GLY      | -      | linker                | UNP O66529 |
| Q     | 41      | SER      | -      | linker                | UNP O66529 |
| Q     | 42      | GLY      | -      | linker                | UNP O66529 |
| Q     | 43      | SER      | -      | linker                | UNP O66529 |
| Q     | 44      | SER      | -      | linker                | UNP O66529 |
| Q     | 45      | MET      | -      | linker                | UNP O66529 |
| Q     | 46      | GLU      | -      | linker                | UNP O66529 |
| R     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| R     | 37      | GLY      | -      | linker                | UNP O66529 |
| R     | 38      | THR      | -      | linker                | UNP O66529 |
| R     | 39      | GLY      | -      | linker                | UNP O66529 |
| R     | 40      | GLY      | -      | linker                | UNP O66529 |
| R     | 41      | SER      | -      | linker                | UNP O66529 |
| R     | 42      | GLY      | -      | linker                | UNP O66529 |
| R     | 43      | SER      | -      | linker                | UNP O66529 |
| R     | 44      | SER      | -      | linker                | UNP O66529 |
| R     | 45      | MET      | -      | linker                | UNP O66529 |
| R     | 46      | GLU      | -      | linker                | UNP O66529 |
| S     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| S     | 37      | GLY      | -      | linker                | UNP O66529 |
| S     | 38      | THR      | -      | linker                | UNP O66529 |
| S     | 39      | GLY      | -      | linker                | UNP O66529 |
| S     | 40      | GLY      | -      | linker                | UNP O66529 |
| S     | 41      | SER      | -      | linker                | UNP O66529 |
| S     | 42      | GLY      | -      | linker                | UNP O66529 |
| S     | 43      | SER      | -      | linker                | UNP O66529 |
| S     | 44      | SER      | -      | linker                | UNP O66529 |
| S     | 45      | MET      | -      | linker                | UNP O66529 |
| S     | 46      | GLU      | -      | linker                | UNP O66529 |
| T     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| T     | 37      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| T     | 38      | THR      | -      | linker                | UNP O66529 |
| T     | 39      | GLY      | -      | linker                | UNP O66529 |
| T     | 40      | GLY      | -      | linker                | UNP O66529 |
| T     | 41      | SER      | -      | linker                | UNP O66529 |
| T     | 42      | GLY      | -      | linker                | UNP O66529 |
| T     | 43      | SER      | -      | linker                | UNP O66529 |
| T     | 44      | SER      | -      | linker                | UNP O66529 |
| T     | 45      | MET      | -      | linker                | UNP O66529 |
| T     | 46      | GLU      | -      | linker                | UNP O66529 |
| U     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| U     | 37      | GLY      | -      | linker                | UNP O66529 |
| U     | 38      | THR      | -      | linker                | UNP O66529 |
| U     | 39      | GLY      | -      | linker                | UNP O66529 |
| U     | 40      | GLY      | -      | linker                | UNP O66529 |
| U     | 41      | SER      | -      | linker                | UNP O66529 |
| U     | 42      | GLY      | -      | linker                | UNP O66529 |
| U     | 43      | SER      | -      | linker                | UNP O66529 |
| U     | 44      | SER      | -      | linker                | UNP O66529 |
| U     | 45      | MET      | -      | linker                | UNP O66529 |
| U     | 46      | GLU      | -      | linker                | UNP O66529 |
| V     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| V     | 37      | GLY      | -      | linker                | UNP O66529 |
| V     | 38      | THR      | -      | linker                | UNP O66529 |
| V     | 39      | GLY      | -      | linker                | UNP O66529 |
| V     | 40      | GLY      | -      | linker                | UNP O66529 |
| V     | 41      | SER      | -      | linker                | UNP O66529 |
| V     | 42      | GLY      | -      | linker                | UNP O66529 |
| V     | 43      | SER      | -      | linker                | UNP O66529 |
| V     | 44      | SER      | -      | linker                | UNP O66529 |
| V     | 45      | MET      | -      | linker                | UNP O66529 |
| V     | 46      | GLU      | -      | linker                | UNP O66529 |
| W     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| W     | 37      | GLY      | -      | linker                | UNP O66529 |
| W     | 38      | THR      | -      | linker                | UNP O66529 |
| W     | 39      | GLY      | -      | linker                | UNP O66529 |
| W     | 40      | GLY      | -      | linker                | UNP O66529 |
| W     | 41      | SER      | -      | linker                | UNP O66529 |
| W     | 42      | GLY      | -      | linker                | UNP O66529 |
| W     | 43      | SER      | -      | linker                | UNP O66529 |
| W     | 44      | SER      | -      | linker                | UNP O66529 |
| W     | 45      | MET      | -      | linker                | UNP O66529 |
| W     | 46      | GLU      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| X     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| X     | 37      | GLY      | -      | linker                | UNP O66529 |
| X     | 38      | THR      | -      | linker                | UNP O66529 |
| X     | 39      | GLY      | -      | linker                | UNP O66529 |
| X     | 40      | GLY      | -      | linker                | UNP O66529 |
| X     | 41      | SER      | -      | linker                | UNP O66529 |
| X     | 42      | GLY      | -      | linker                | UNP O66529 |
| X     | 43      | SER      | -      | linker                | UNP O66529 |
| X     | 44      | SER      | -      | linker                | UNP O66529 |
| X     | 45      | MET      | -      | linker                | UNP O66529 |
| X     | 46      | GLU      | -      | linker                | UNP O66529 |
| Y     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| Y     | 37      | GLY      | -      | linker                | UNP O66529 |
| Y     | 38      | THR      | -      | linker                | UNP O66529 |
| Y     | 39      | GLY      | -      | linker                | UNP O66529 |
| Y     | 40      | GLY      | -      | linker                | UNP O66529 |
| Y     | 41      | SER      | -      | linker                | UNP O66529 |
| Y     | 42      | GLY      | -      | linker                | UNP O66529 |
| Y     | 43      | SER      | -      | linker                | UNP O66529 |
| Y     | 44      | SER      | -      | linker                | UNP O66529 |
| Y     | 45      | MET      | -      | linker                | UNP O66529 |
| Y     | 46      | GLU      | -      | linker                | UNP O66529 |
| Z     | 1       | MET      | -      | initiating methionine | UNP O66529 |
| Z     | 37      | GLY      | -      | linker                | UNP O66529 |
| Z     | 38      | THR      | -      | linker                | UNP O66529 |
| Z     | 39      | GLY      | -      | linker                | UNP O66529 |
| Z     | 40      | GLY      | -      | linker                | UNP O66529 |
| Z     | 41      | SER      | -      | linker                | UNP O66529 |
| Z     | 42      | GLY      | -      | linker                | UNP O66529 |
| Z     | 43      | SER      | -      | linker                | UNP O66529 |
| Z     | 44      | SER      | -      | linker                | UNP O66529 |
| Z     | 45      | MET      | -      | linker                | UNP O66529 |
| Z     | 46      | GLU      | -      | linker                | UNP O66529 |
| AA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| AA    | 37      | GLY      | -      | linker                | UNP O66529 |
| AA    | 38      | THR      | -      | linker                | UNP O66529 |
| AA    | 39      | GLY      | -      | linker                | UNP O66529 |
| AA    | 40      | GLY      | -      | linker                | UNP O66529 |
| AA    | 41      | SER      | -      | linker                | UNP O66529 |
| AA    | 42      | GLY      | -      | linker                | UNP O66529 |
| AA    | 43      | SER      | -      | linker                | UNP O66529 |
| AA    | 44      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| AA    | 45      | MET      | -      | linker                | UNP O66529 |
| AA    | 46      | GLU      | -      | linker                | UNP O66529 |
| BA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| BA    | 37      | GLY      | -      | linker                | UNP O66529 |
| BA    | 38      | THR      | -      | linker                | UNP O66529 |
| BA    | 39      | GLY      | -      | linker                | UNP O66529 |
| BA    | 40      | GLY      | -      | linker                | UNP O66529 |
| BA    | 41      | SER      | -      | linker                | UNP O66529 |
| BA    | 42      | GLY      | -      | linker                | UNP O66529 |
| BA    | 43      | SER      | -      | linker                | UNP O66529 |
| BA    | 44      | SER      | -      | linker                | UNP O66529 |
| BA    | 45      | MET      | -      | linker                | UNP O66529 |
| BA    | 46      | GLU      | -      | linker                | UNP O66529 |
| CA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| CA    | 37      | GLY      | -      | linker                | UNP O66529 |
| CA    | 38      | THR      | -      | linker                | UNP O66529 |
| CA    | 39      | GLY      | -      | linker                | UNP O66529 |
| CA    | 40      | GLY      | -      | linker                | UNP O66529 |
| CA    | 41      | SER      | -      | linker                | UNP O66529 |
| CA    | 42      | GLY      | -      | linker                | UNP O66529 |
| CA    | 43      | SER      | -      | linker                | UNP O66529 |
| CA    | 44      | SER      | -      | linker                | UNP O66529 |
| CA    | 45      | MET      | -      | linker                | UNP O66529 |
| CA    | 46      | GLU      | -      | linker                | UNP O66529 |
| DA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| DA    | 37      | GLY      | -      | linker                | UNP O66529 |
| DA    | 38      | THR      | -      | linker                | UNP O66529 |
| DA    | 39      | GLY      | -      | linker                | UNP O66529 |
| DA    | 40      | GLY      | -      | linker                | UNP O66529 |
| DA    | 41      | SER      | -      | linker                | UNP O66529 |
| DA    | 42      | GLY      | -      | linker                | UNP O66529 |
| DA    | 43      | SER      | -      | linker                | UNP O66529 |
| DA    | 44      | SER      | -      | linker                | UNP O66529 |
| DA    | 45      | MET      | -      | linker                | UNP O66529 |
| DA    | 46      | GLU      | -      | linker                | UNP O66529 |
| EA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| EA    | 37      | GLY      | -      | linker                | UNP O66529 |
| EA    | 38      | THR      | -      | linker                | UNP O66529 |
| EA    | 39      | GLY      | -      | linker                | UNP O66529 |
| EA    | 40      | GLY      | -      | linker                | UNP O66529 |
| EA    | 41      | SER      | -      | linker                | UNP O66529 |
| EA    | 42      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| EA    | 43      | SER      | -      | linker                | UNP O66529 |
| EA    | 44      | SER      | -      | linker                | UNP O66529 |
| EA    | 45      | MET      | -      | linker                | UNP O66529 |
| EA    | 46      | GLU      | -      | linker                | UNP O66529 |
| FA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| FA    | 37      | GLY      | -      | linker                | UNP O66529 |
| FA    | 38      | THR      | -      | linker                | UNP O66529 |
| FA    | 39      | GLY      | -      | linker                | UNP O66529 |
| FA    | 40      | GLY      | -      | linker                | UNP O66529 |
| FA    | 41      | SER      | -      | linker                | UNP O66529 |
| FA    | 42      | GLY      | -      | linker                | UNP O66529 |
| FA    | 43      | SER      | -      | linker                | UNP O66529 |
| FA    | 44      | SER      | -      | linker                | UNP O66529 |
| FA    | 45      | MET      | -      | linker                | UNP O66529 |
| FA    | 46      | GLU      | -      | linker                | UNP O66529 |
| GA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| GA    | 37      | GLY      | -      | linker                | UNP O66529 |
| GA    | 38      | THR      | -      | linker                | UNP O66529 |
| GA    | 39      | GLY      | -      | linker                | UNP O66529 |
| GA    | 40      | GLY      | -      | linker                | UNP O66529 |
| GA    | 41      | SER      | -      | linker                | UNP O66529 |
| GA    | 42      | GLY      | -      | linker                | UNP O66529 |
| GA    | 43      | SER      | -      | linker                | UNP O66529 |
| GA    | 44      | SER      | -      | linker                | UNP O66529 |
| GA    | 45      | MET      | -      | linker                | UNP O66529 |
| GA    | 46      | GLU      | -      | linker                | UNP O66529 |
| HA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| HA    | 37      | GLY      | -      | linker                | UNP O66529 |
| HA    | 38      | THR      | -      | linker                | UNP O66529 |
| HA    | 39      | GLY      | -      | linker                | UNP O66529 |
| HA    | 40      | GLY      | -      | linker                | UNP O66529 |
| HA    | 41      | SER      | -      | linker                | UNP O66529 |
| HA    | 42      | GLY      | -      | linker                | UNP O66529 |
| HA    | 43      | SER      | -      | linker                | UNP O66529 |
| HA    | 44      | SER      | -      | linker                | UNP O66529 |
| HA    | 45      | MET      | -      | linker                | UNP O66529 |
| HA    | 46      | GLU      | -      | linker                | UNP O66529 |
| IA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| IA    | 37      | GLY      | -      | linker                | UNP O66529 |
| IA    | 38      | THR      | -      | linker                | UNP O66529 |
| IA    | 39      | GLY      | -      | linker                | UNP O66529 |
| IA    | 40      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| IA    | 41      | SER      | -      | linker                | UNP O66529 |
| IA    | 42      | GLY      | -      | linker                | UNP O66529 |
| IA    | 43      | SER      | -      | linker                | UNP O66529 |
| IA    | 44      | SER      | -      | linker                | UNP O66529 |
| IA    | 45      | MET      | -      | linker                | UNP O66529 |
| IA    | 46      | GLU      | -      | linker                | UNP O66529 |
| JA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| JA    | 37      | GLY      | -      | linker                | UNP O66529 |
| JA    | 38      | THR      | -      | linker                | UNP O66529 |
| JA    | 39      | GLY      | -      | linker                | UNP O66529 |
| JA    | 40      | GLY      | -      | linker                | UNP O66529 |
| JA    | 41      | SER      | -      | linker                | UNP O66529 |
| JA    | 42      | GLY      | -      | linker                | UNP O66529 |
| JA    | 43      | SER      | -      | linker                | UNP O66529 |
| JA    | 44      | SER      | -      | linker                | UNP O66529 |
| JA    | 45      | MET      | -      | linker                | UNP O66529 |
| JA    | 46      | GLU      | -      | linker                | UNP O66529 |
| KA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| KA    | 37      | GLY      | -      | linker                | UNP O66529 |
| KA    | 38      | THR      | -      | linker                | UNP O66529 |
| KA    | 39      | GLY      | -      | linker                | UNP O66529 |
| KA    | 40      | GLY      | -      | linker                | UNP O66529 |
| KA    | 41      | SER      | -      | linker                | UNP O66529 |
| KA    | 42      | GLY      | -      | linker                | UNP O66529 |
| KA    | 43      | SER      | -      | linker                | UNP O66529 |
| KA    | 44      | SER      | -      | linker                | UNP O66529 |
| KA    | 45      | MET      | -      | linker                | UNP O66529 |
| KA    | 46      | GLU      | -      | linker                | UNP O66529 |
| LA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| LA    | 37      | GLY      | -      | linker                | UNP O66529 |
| LA    | 38      | THR      | -      | linker                | UNP O66529 |
| LA    | 39      | GLY      | -      | linker                | UNP O66529 |
| LA    | 40      | GLY      | -      | linker                | UNP O66529 |
| LA    | 41      | SER      | -      | linker                | UNP O66529 |
| LA    | 42      | GLY      | -      | linker                | UNP O66529 |
| LA    | 43      | SER      | -      | linker                | UNP O66529 |
| LA    | 44      | SER      | -      | linker                | UNP O66529 |
| LA    | 45      | MET      | -      | linker                | UNP O66529 |
| LA    | 46      | GLU      | -      | linker                | UNP O66529 |
| MA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| MA    | 37      | GLY      | -      | linker                | UNP O66529 |
| MA    | 38      | THR      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| MA    | 39      | GLY      | -      | linker                | UNP O66529 |
| MA    | 40      | GLY      | -      | linker                | UNP O66529 |
| MA    | 41      | SER      | -      | linker                | UNP O66529 |
| MA    | 42      | GLY      | -      | linker                | UNP O66529 |
| MA    | 43      | SER      | -      | linker                | UNP O66529 |
| MA    | 44      | SER      | -      | linker                | UNP O66529 |
| MA    | 45      | MET      | -      | linker                | UNP O66529 |
| MA    | 46      | GLU      | -      | linker                | UNP O66529 |
| NA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| NA    | 37      | GLY      | -      | linker                | UNP O66529 |
| NA    | 38      | THR      | -      | linker                | UNP O66529 |
| NA    | 39      | GLY      | -      | linker                | UNP O66529 |
| NA    | 40      | GLY      | -      | linker                | UNP O66529 |
| NA    | 41      | SER      | -      | linker                | UNP O66529 |
| NA    | 42      | GLY      | -      | linker                | UNP O66529 |
| NA    | 43      | SER      | -      | linker                | UNP O66529 |
| NA    | 44      | SER      | -      | linker                | UNP O66529 |
| NA    | 45      | MET      | -      | linker                | UNP O66529 |
| NA    | 46      | GLU      | -      | linker                | UNP O66529 |
| OA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| OA    | 37      | GLY      | -      | linker                | UNP O66529 |
| OA    | 38      | THR      | -      | linker                | UNP O66529 |
| OA    | 39      | GLY      | -      | linker                | UNP O66529 |
| OA    | 40      | GLY      | -      | linker                | UNP O66529 |
| OA    | 41      | SER      | -      | linker                | UNP O66529 |
| OA    | 42      | GLY      | -      | linker                | UNP O66529 |
| OA    | 43      | SER      | -      | linker                | UNP O66529 |
| OA    | 44      | SER      | -      | linker                | UNP O66529 |
| OA    | 45      | MET      | -      | linker                | UNP O66529 |
| OA    | 46      | GLU      | -      | linker                | UNP O66529 |
| PA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| PA    | 37      | GLY      | -      | linker                | UNP O66529 |
| PA    | 38      | THR      | -      | linker                | UNP O66529 |
| PA    | 39      | GLY      | -      | linker                | UNP O66529 |
| PA    | 40      | GLY      | -      | linker                | UNP O66529 |
| PA    | 41      | SER      | -      | linker                | UNP O66529 |
| PA    | 42      | GLY      | -      | linker                | UNP O66529 |
| PA    | 43      | SER      | -      | linker                | UNP O66529 |
| PA    | 44      | SER      | -      | linker                | UNP O66529 |
| PA    | 45      | MET      | -      | linker                | UNP O66529 |
| PA    | 46      | GLU      | -      | linker                | UNP O66529 |
| QA    | 1       | MET      | -      | initiating methionine | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| QA    | 37      | GLY      | -      | linker                | UNP O66529 |
| QA    | 38      | THR      | -      | linker                | UNP O66529 |
| QA    | 39      | GLY      | -      | linker                | UNP O66529 |
| QA    | 40      | GLY      | -      | linker                | UNP O66529 |
| QA    | 41      | SER      | -      | linker                | UNP O66529 |
| QA    | 42      | GLY      | -      | linker                | UNP O66529 |
| QA    | 43      | SER      | -      | linker                | UNP O66529 |
| QA    | 44      | SER      | -      | linker                | UNP O66529 |
| QA    | 45      | MET      | -      | linker                | UNP O66529 |
| QA    | 46      | GLU      | -      | linker                | UNP O66529 |
| RA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| RA    | 37      | GLY      | -      | linker                | UNP O66529 |
| RA    | 38      | THR      | -      | linker                | UNP O66529 |
| RA    | 39      | GLY      | -      | linker                | UNP O66529 |
| RA    | 40      | GLY      | -      | linker                | UNP O66529 |
| RA    | 41      | SER      | -      | linker                | UNP O66529 |
| RA    | 42      | GLY      | -      | linker                | UNP O66529 |
| RA    | 43      | SER      | -      | linker                | UNP O66529 |
| RA    | 44      | SER      | -      | linker                | UNP O66529 |
| RA    | 45      | MET      | -      | linker                | UNP O66529 |
| RA    | 46      | GLU      | -      | linker                | UNP O66529 |
| SA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| SA    | 37      | GLY      | -      | linker                | UNP O66529 |
| SA    | 38      | THR      | -      | linker                | UNP O66529 |
| SA    | 39      | GLY      | -      | linker                | UNP O66529 |
| SA    | 40      | GLY      | -      | linker                | UNP O66529 |
| SA    | 41      | SER      | -      | linker                | UNP O66529 |
| SA    | 42      | GLY      | -      | linker                | UNP O66529 |
| SA    | 43      | SER      | -      | linker                | UNP O66529 |
| SA    | 44      | SER      | -      | linker                | UNP O66529 |
| SA    | 45      | MET      | -      | linker                | UNP O66529 |
| SA    | 46      | GLU      | -      | linker                | UNP O66529 |
| TA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| TA    | 37      | GLY      | -      | linker                | UNP O66529 |
| TA    | 38      | THR      | -      | linker                | UNP O66529 |
| TA    | 39      | GLY      | -      | linker                | UNP O66529 |
| TA    | 40      | GLY      | -      | linker                | UNP O66529 |
| TA    | 41      | SER      | -      | linker                | UNP O66529 |
| TA    | 42      | GLY      | -      | linker                | UNP O66529 |
| TA    | 43      | SER      | -      | linker                | UNP O66529 |
| TA    | 44      | SER      | -      | linker                | UNP O66529 |
| TA    | 45      | MET      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| TA    | 46      | GLU      | -      | linker                | UNP O66529 |
| UA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| UA    | 37      | GLY      | -      | linker                | UNP O66529 |
| UA    | 38      | THR      | -      | linker                | UNP O66529 |
| UA    | 39      | GLY      | -      | linker                | UNP O66529 |
| UA    | 40      | GLY      | -      | linker                | UNP O66529 |
| UA    | 41      | SER      | -      | linker                | UNP O66529 |
| UA    | 42      | GLY      | -      | linker                | UNP O66529 |
| UA    | 43      | SER      | -      | linker                | UNP O66529 |
| UA    | 44      | SER      | -      | linker                | UNP O66529 |
| UA    | 45      | MET      | -      | linker                | UNP O66529 |
| UA    | 46      | GLU      | -      | linker                | UNP O66529 |
| VA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| VA    | 37      | GLY      | -      | linker                | UNP O66529 |
| VA    | 38      | THR      | -      | linker                | UNP O66529 |
| VA    | 39      | GLY      | -      | linker                | UNP O66529 |
| VA    | 40      | GLY      | -      | linker                | UNP O66529 |
| VA    | 41      | SER      | -      | linker                | UNP O66529 |
| VA    | 42      | GLY      | -      | linker                | UNP O66529 |
| VA    | 43      | SER      | -      | linker                | UNP O66529 |
| VA    | 44      | SER      | -      | linker                | UNP O66529 |
| VA    | 45      | MET      | -      | linker                | UNP O66529 |
| VA    | 46      | GLU      | -      | linker                | UNP O66529 |
| WA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| WA    | 37      | GLY      | -      | linker                | UNP O66529 |
| WA    | 38      | THR      | -      | linker                | UNP O66529 |
| WA    | 39      | GLY      | -      | linker                | UNP O66529 |
| WA    | 40      | GLY      | -      | linker                | UNP O66529 |
| WA    | 41      | SER      | -      | linker                | UNP O66529 |
| WA    | 42      | GLY      | -      | linker                | UNP O66529 |
| WA    | 43      | SER      | -      | linker                | UNP O66529 |
| WA    | 44      | SER      | -      | linker                | UNP O66529 |
| WA    | 45      | MET      | -      | linker                | UNP O66529 |
| WA    | 46      | GLU      | -      | linker                | UNP O66529 |
| XA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| XA    | 37      | GLY      | -      | linker                | UNP O66529 |
| XA    | 38      | THR      | -      | linker                | UNP O66529 |
| XA    | 39      | GLY      | -      | linker                | UNP O66529 |
| XA    | 40      | GLY      | -      | linker                | UNP O66529 |
| XA    | 41      | SER      | -      | linker                | UNP O66529 |
| XA    | 42      | GLY      | -      | linker                | UNP O66529 |
| XA    | 43      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| XA    | 44      | SER      | -      | linker                | UNP O66529 |
| XA    | 45      | MET      | -      | linker                | UNP O66529 |
| XA    | 46      | GLU      | -      | linker                | UNP O66529 |
| YA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| YA    | 37      | GLY      | -      | linker                | UNP O66529 |
| YA    | 38      | THR      | -      | linker                | UNP O66529 |
| YA    | 39      | GLY      | -      | linker                | UNP O66529 |
| YA    | 40      | GLY      | -      | linker                | UNP O66529 |
| YA    | 41      | SER      | -      | linker                | UNP O66529 |
| YA    | 42      | GLY      | -      | linker                | UNP O66529 |
| YA    | 43      | SER      | -      | linker                | UNP O66529 |
| YA    | 44      | SER      | -      | linker                | UNP O66529 |
| YA    | 45      | MET      | -      | linker                | UNP O66529 |
| YA    | 46      | GLU      | -      | linker                | UNP O66529 |
| ZA    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| ZA    | 37      | GLY      | -      | linker                | UNP O66529 |
| ZA    | 38      | THR      | -      | linker                | UNP O66529 |
| ZA    | 39      | GLY      | -      | linker                | UNP O66529 |
| ZA    | 40      | GLY      | -      | linker                | UNP O66529 |
| ZA    | 41      | SER      | -      | linker                | UNP O66529 |
| ZA    | 42      | GLY      | -      | linker                | UNP O66529 |
| ZA    | 43      | SER      | -      | linker                | UNP O66529 |
| ZA    | 44      | SER      | -      | linker                | UNP O66529 |
| ZA    | 45      | MET      | -      | linker                | UNP O66529 |
| ZA    | 46      | GLU      | -      | linker                | UNP O66529 |
| AB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| AB    | 37      | GLY      | -      | linker                | UNP O66529 |
| AB    | 38      | THR      | -      | linker                | UNP O66529 |
| AB    | 39      | GLY      | -      | linker                | UNP O66529 |
| AB    | 40      | GLY      | -      | linker                | UNP O66529 |
| AB    | 41      | SER      | -      | linker                | UNP O66529 |
| AB    | 42      | GLY      | -      | linker                | UNP O66529 |
| AB    | 43      | SER      | -      | linker                | UNP O66529 |
| AB    | 44      | SER      | -      | linker                | UNP O66529 |
| AB    | 45      | MET      | -      | linker                | UNP O66529 |
| AB    | 46      | GLU      | -      | linker                | UNP O66529 |
| BB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| BB    | 37      | GLY      | -      | linker                | UNP O66529 |
| BB    | 38      | THR      | -      | linker                | UNP O66529 |
| BB    | 39      | GLY      | -      | linker                | UNP O66529 |
| BB    | 40      | GLY      | -      | linker                | UNP O66529 |
| BB    | 41      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| BB    | 42      | GLY      | -      | linker                | UNP O66529 |
| BB    | 43      | SER      | -      | linker                | UNP O66529 |
| BB    | 44      | SER      | -      | linker                | UNP O66529 |
| BB    | 45      | MET      | -      | linker                | UNP O66529 |
| BB    | 46      | GLU      | -      | linker                | UNP O66529 |
| CB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| CB    | 37      | GLY      | -      | linker                | UNP O66529 |
| CB    | 38      | THR      | -      | linker                | UNP O66529 |
| CB    | 39      | GLY      | -      | linker                | UNP O66529 |
| CB    | 40      | GLY      | -      | linker                | UNP O66529 |
| CB    | 41      | SER      | -      | linker                | UNP O66529 |
| CB    | 42      | GLY      | -      | linker                | UNP O66529 |
| CB    | 43      | SER      | -      | linker                | UNP O66529 |
| CB    | 44      | SER      | -      | linker                | UNP O66529 |
| CB    | 45      | MET      | -      | linker                | UNP O66529 |
| CB    | 46      | GLU      | -      | linker                | UNP O66529 |
| DB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| DB    | 37      | GLY      | -      | linker                | UNP O66529 |
| DB    | 38      | THR      | -      | linker                | UNP O66529 |
| DB    | 39      | GLY      | -      | linker                | UNP O66529 |
| DB    | 40      | GLY      | -      | linker                | UNP O66529 |
| DB    | 41      | SER      | -      | linker                | UNP O66529 |
| DB    | 42      | GLY      | -      | linker                | UNP O66529 |
| DB    | 43      | SER      | -      | linker                | UNP O66529 |
| DB    | 44      | SER      | -      | linker                | UNP O66529 |
| DB    | 45      | MET      | -      | linker                | UNP O66529 |
| DB    | 46      | GLU      | -      | linker                | UNP O66529 |
| EB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| EB    | 37      | GLY      | -      | linker                | UNP O66529 |
| EB    | 38      | THR      | -      | linker                | UNP O66529 |
| EB    | 39      | GLY      | -      | linker                | UNP O66529 |
| EB    | 40      | GLY      | -      | linker                | UNP O66529 |
| EB    | 41      | SER      | -      | linker                | UNP O66529 |
| EB    | 42      | GLY      | -      | linker                | UNP O66529 |
| EB    | 43      | SER      | -      | linker                | UNP O66529 |
| EB    | 44      | SER      | -      | linker                | UNP O66529 |
| EB    | 45      | MET      | -      | linker                | UNP O66529 |
| EB    | 46      | GLU      | -      | linker                | UNP O66529 |
| FB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| FB    | 37      | GLY      | -      | linker                | UNP O66529 |
| FB    | 38      | THR      | -      | linker                | UNP O66529 |
| FB    | 39      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| FB    | 40      | GLY      | -      | linker                | UNP O66529 |
| FB    | 41      | SER      | -      | linker                | UNP O66529 |
| FB    | 42      | GLY      | -      | linker                | UNP O66529 |
| FB    | 43      | SER      | -      | linker                | UNP O66529 |
| FB    | 44      | SER      | -      | linker                | UNP O66529 |
| FB    | 45      | MET      | -      | linker                | UNP O66529 |
| FB    | 46      | GLU      | -      | linker                | UNP O66529 |
| GB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| GB    | 37      | GLY      | -      | linker                | UNP O66529 |
| GB    | 38      | THR      | -      | linker                | UNP O66529 |
| GB    | 39      | GLY      | -      | linker                | UNP O66529 |
| GB    | 40      | GLY      | -      | linker                | UNP O66529 |
| GB    | 41      | SER      | -      | linker                | UNP O66529 |
| GB    | 42      | GLY      | -      | linker                | UNP O66529 |
| GB    | 43      | SER      | -      | linker                | UNP O66529 |
| GB    | 44      | SER      | -      | linker                | UNP O66529 |
| GB    | 45      | MET      | -      | linker                | UNP O66529 |
| GB    | 46      | GLU      | -      | linker                | UNP O66529 |
| HB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| HB    | 37      | GLY      | -      | linker                | UNP O66529 |
| HB    | 38      | THR      | -      | linker                | UNP O66529 |
| HB    | 39      | GLY      | -      | linker                | UNP O66529 |
| HB    | 40      | GLY      | -      | linker                | UNP O66529 |
| HB    | 41      | SER      | -      | linker                | UNP O66529 |
| HB    | 42      | GLY      | -      | linker                | UNP O66529 |
| HB    | 43      | SER      | -      | linker                | UNP O66529 |
| HB    | 44      | SER      | -      | linker                | UNP O66529 |
| HB    | 45      | MET      | -      | linker                | UNP O66529 |
| HB    | 46      | GLU      | -      | linker                | UNP O66529 |
| IB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| IB    | 37      | GLY      | -      | linker                | UNP O66529 |
| IB    | 38      | THR      | -      | linker                | UNP O66529 |
| IB    | 39      | GLY      | -      | linker                | UNP O66529 |
| IB    | 40      | GLY      | -      | linker                | UNP O66529 |
| IB    | 41      | SER      | -      | linker                | UNP O66529 |
| IB    | 42      | GLY      | -      | linker                | UNP O66529 |
| IB    | 43      | SER      | -      | linker                | UNP O66529 |
| IB    | 44      | SER      | -      | linker                | UNP O66529 |
| IB    | 45      | MET      | -      | linker                | UNP O66529 |
| IB    | 46      | GLU      | -      | linker                | UNP O66529 |
| JB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| JB    | 37      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| JB    | 38      | THR      | -      | linker                | UNP O66529 |
| JB    | 39      | GLY      | -      | linker                | UNP O66529 |
| JB    | 40      | GLY      | -      | linker                | UNP O66529 |
| JB    | 41      | SER      | -      | linker                | UNP O66529 |
| JB    | 42      | GLY      | -      | linker                | UNP O66529 |
| JB    | 43      | SER      | -      | linker                | UNP O66529 |
| JB    | 44      | SER      | -      | linker                | UNP O66529 |
| JB    | 45      | MET      | -      | linker                | UNP O66529 |
| JB    | 46      | GLU      | -      | linker                | UNP O66529 |
| KB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| KB    | 37      | GLY      | -      | linker                | UNP O66529 |
| KB    | 38      | THR      | -      | linker                | UNP O66529 |
| KB    | 39      | GLY      | -      | linker                | UNP O66529 |
| KB    | 40      | GLY      | -      | linker                | UNP O66529 |
| KB    | 41      | SER      | -      | linker                | UNP O66529 |
| KB    | 42      | GLY      | -      | linker                | UNP O66529 |
| KB    | 43      | SER      | -      | linker                | UNP O66529 |
| KB    | 44      | SER      | -      | linker                | UNP O66529 |
| KB    | 45      | MET      | -      | linker                | UNP O66529 |
| KB    | 46      | GLU      | -      | linker                | UNP O66529 |
| LB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| LB    | 37      | GLY      | -      | linker                | UNP O66529 |
| LB    | 38      | THR      | -      | linker                | UNP O66529 |
| LB    | 39      | GLY      | -      | linker                | UNP O66529 |
| LB    | 40      | GLY      | -      | linker                | UNP O66529 |
| LB    | 41      | SER      | -      | linker                | UNP O66529 |
| LB    | 42      | GLY      | -      | linker                | UNP O66529 |
| LB    | 43      | SER      | -      | linker                | UNP O66529 |
| LB    | 44      | SER      | -      | linker                | UNP O66529 |
| LB    | 45      | MET      | -      | linker                | UNP O66529 |
| LB    | 46      | GLU      | -      | linker                | UNP O66529 |
| MB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| MB    | 37      | GLY      | -      | linker                | UNP O66529 |
| MB    | 38      | THR      | -      | linker                | UNP O66529 |
| MB    | 39      | GLY      | -      | linker                | UNP O66529 |
| MB    | 40      | GLY      | -      | linker                | UNP O66529 |
| MB    | 41      | SER      | -      | linker                | UNP O66529 |
| MB    | 42      | GLY      | -      | linker                | UNP O66529 |
| MB    | 43      | SER      | -      | linker                | UNP O66529 |
| MB    | 44      | SER      | -      | linker                | UNP O66529 |
| MB    | 45      | MET      | -      | linker                | UNP O66529 |
| MB    | 46      | GLU      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| NB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| NB    | 37      | GLY      | -      | linker                | UNP O66529 |
| NB    | 38      | THR      | -      | linker                | UNP O66529 |
| NB    | 39      | GLY      | -      | linker                | UNP O66529 |
| NB    | 40      | GLY      | -      | linker                | UNP O66529 |
| NB    | 41      | SER      | -      | linker                | UNP O66529 |
| NB    | 42      | GLY      | -      | linker                | UNP O66529 |
| NB    | 43      | SER      | -      | linker                | UNP O66529 |
| NB    | 44      | SER      | -      | linker                | UNP O66529 |
| NB    | 45      | MET      | -      | linker                | UNP O66529 |
| NB    | 46      | GLU      | -      | linker                | UNP O66529 |
| OB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| OB    | 37      | GLY      | -      | linker                | UNP O66529 |
| OB    | 38      | THR      | -      | linker                | UNP O66529 |
| OB    | 39      | GLY      | -      | linker                | UNP O66529 |
| OB    | 40      | GLY      | -      | linker                | UNP O66529 |
| OB    | 41      | SER      | -      | linker                | UNP O66529 |
| OB    | 42      | GLY      | -      | linker                | UNP O66529 |
| OB    | 43      | SER      | -      | linker                | UNP O66529 |
| OB    | 44      | SER      | -      | linker                | UNP O66529 |
| OB    | 45      | MET      | -      | linker                | UNP O66529 |
| OB    | 46      | GLU      | -      | linker                | UNP O66529 |
| PB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| PB    | 37      | GLY      | -      | linker                | UNP O66529 |
| PB    | 38      | THR      | -      | linker                | UNP O66529 |
| PB    | 39      | GLY      | -      | linker                | UNP O66529 |
| PB    | 40      | GLY      | -      | linker                | UNP O66529 |
| PB    | 41      | SER      | -      | linker                | UNP O66529 |
| PB    | 42      | GLY      | -      | linker                | UNP O66529 |
| PB    | 43      | SER      | -      | linker                | UNP O66529 |
| PB    | 44      | SER      | -      | linker                | UNP O66529 |
| PB    | 45      | MET      | -      | linker                | UNP O66529 |
| PB    | 46      | GLU      | -      | linker                | UNP O66529 |
| QB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| QB    | 37      | GLY      | -      | linker                | UNP O66529 |
| QB    | 38      | THR      | -      | linker                | UNP O66529 |
| QB    | 39      | GLY      | -      | linker                | UNP O66529 |
| QB    | 40      | GLY      | -      | linker                | UNP O66529 |
| QB    | 41      | SER      | -      | linker                | UNP O66529 |
| QB    | 42      | GLY      | -      | linker                | UNP O66529 |
| QB    | 43      | SER      | -      | linker                | UNP O66529 |
| QB    | 44      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| QB    | 45      | MET      | -      | linker                | UNP O66529 |
| QB    | 46      | GLU      | -      | linker                | UNP O66529 |
| RB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| RB    | 37      | GLY      | -      | linker                | UNP O66529 |
| RB    | 38      | THR      | -      | linker                | UNP O66529 |
| RB    | 39      | GLY      | -      | linker                | UNP O66529 |
| RB    | 40      | GLY      | -      | linker                | UNP O66529 |
| RB    | 41      | SER      | -      | linker                | UNP O66529 |
| RB    | 42      | GLY      | -      | linker                | UNP O66529 |
| RB    | 43      | SER      | -      | linker                | UNP O66529 |
| RB    | 44      | SER      | -      | linker                | UNP O66529 |
| RB    | 45      | MET      | -      | linker                | UNP O66529 |
| RB    | 46      | GLU      | -      | linker                | UNP O66529 |
| SB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| SB    | 37      | GLY      | -      | linker                | UNP O66529 |
| SB    | 38      | THR      | -      | linker                | UNP O66529 |
| SB    | 39      | GLY      | -      | linker                | UNP O66529 |
| SB    | 40      | GLY      | -      | linker                | UNP O66529 |
| SB    | 41      | SER      | -      | linker                | UNP O66529 |
| SB    | 42      | GLY      | -      | linker                | UNP O66529 |
| SB    | 43      | SER      | -      | linker                | UNP O66529 |
| SB    | 44      | SER      | -      | linker                | UNP O66529 |
| SB    | 45      | MET      | -      | linker                | UNP O66529 |
| SB    | 46      | GLU      | -      | linker                | UNP O66529 |
| TB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| TB    | 37      | GLY      | -      | linker                | UNP O66529 |
| TB    | 38      | THR      | -      | linker                | UNP O66529 |
| TB    | 39      | GLY      | -      | linker                | UNP O66529 |
| TB    | 40      | GLY      | -      | linker                | UNP O66529 |
| TB    | 41      | SER      | -      | linker                | UNP O66529 |
| TB    | 42      | GLY      | -      | linker                | UNP O66529 |
| TB    | 43      | SER      | -      | linker                | UNP O66529 |
| TB    | 44      | SER      | -      | linker                | UNP O66529 |
| TB    | 45      | MET      | -      | linker                | UNP O66529 |
| TB    | 46      | GLU      | -      | linker                | UNP O66529 |
| UB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| UB    | 37      | GLY      | -      | linker                | UNP O66529 |
| UB    | 38      | THR      | -      | linker                | UNP O66529 |
| UB    | 39      | GLY      | -      | linker                | UNP O66529 |
| UB    | 40      | GLY      | -      | linker                | UNP O66529 |
| UB    | 41      | SER      | -      | linker                | UNP O66529 |
| UB    | 42      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| UB    | 43      | SER      | -      | linker                | UNP O66529 |
| UB    | 44      | SER      | -      | linker                | UNP O66529 |
| UB    | 45      | MET      | -      | linker                | UNP O66529 |
| UB    | 46      | GLU      | -      | linker                | UNP O66529 |
| VB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| VB    | 37      | GLY      | -      | linker                | UNP O66529 |
| VB    | 38      | THR      | -      | linker                | UNP O66529 |
| VB    | 39      | GLY      | -      | linker                | UNP O66529 |
| VB    | 40      | GLY      | -      | linker                | UNP O66529 |
| VB    | 41      | SER      | -      | linker                | UNP O66529 |
| VB    | 42      | GLY      | -      | linker                | UNP O66529 |
| VB    | 43      | SER      | -      | linker                | UNP O66529 |
| VB    | 44      | SER      | -      | linker                | UNP O66529 |
| VB    | 45      | MET      | -      | linker                | UNP O66529 |
| VB    | 46      | GLU      | -      | linker                | UNP O66529 |
| WB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| WB    | 37      | GLY      | -      | linker                | UNP O66529 |
| WB    | 38      | THR      | -      | linker                | UNP O66529 |
| WB    | 39      | GLY      | -      | linker                | UNP O66529 |
| WB    | 40      | GLY      | -      | linker                | UNP O66529 |
| WB    | 41      | SER      | -      | linker                | UNP O66529 |
| WB    | 42      | GLY      | -      | linker                | UNP O66529 |
| WB    | 43      | SER      | -      | linker                | UNP O66529 |
| WB    | 44      | SER      | -      | linker                | UNP O66529 |
| WB    | 45      | MET      | -      | linker                | UNP O66529 |
| WB    | 46      | GLU      | -      | linker                | UNP O66529 |
| XB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| XB    | 37      | GLY      | -      | linker                | UNP O66529 |
| XB    | 38      | THR      | -      | linker                | UNP O66529 |
| XB    | 39      | GLY      | -      | linker                | UNP O66529 |
| XB    | 40      | GLY      | -      | linker                | UNP O66529 |
| XB    | 41      | SER      | -      | linker                | UNP O66529 |
| XB    | 42      | GLY      | -      | linker                | UNP O66529 |
| XB    | 43      | SER      | -      | linker                | UNP O66529 |
| XB    | 44      | SER      | -      | linker                | UNP O66529 |
| XB    | 45      | MET      | -      | linker                | UNP O66529 |
| XB    | 46      | GLU      | -      | linker                | UNP O66529 |
| YB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| YB    | 37      | GLY      | -      | linker                | UNP O66529 |
| YB    | 38      | THR      | -      | linker                | UNP O66529 |
| YB    | 39      | GLY      | -      | linker                | UNP O66529 |
| YB    | 40      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| YB    | 41      | SER      | -      | linker                | UNP O66529 |
| YB    | 42      | GLY      | -      | linker                | UNP O66529 |
| YB    | 43      | SER      | -      | linker                | UNP O66529 |
| YB    | 44      | SER      | -      | linker                | UNP O66529 |
| YB    | 45      | MET      | -      | linker                | UNP O66529 |
| YB    | 46      | GLU      | -      | linker                | UNP O66529 |
| ZB    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| ZB    | 37      | GLY      | -      | linker                | UNP O66529 |
| ZB    | 38      | THR      | -      | linker                | UNP O66529 |
| ZB    | 39      | GLY      | -      | linker                | UNP O66529 |
| ZB    | 40      | GLY      | -      | linker                | UNP O66529 |
| ZB    | 41      | SER      | -      | linker                | UNP O66529 |
| ZB    | 42      | GLY      | -      | linker                | UNP O66529 |
| ZB    | 43      | SER      | -      | linker                | UNP O66529 |
| ZB    | 44      | SER      | -      | linker                | UNP O66529 |
| ZB    | 45      | MET      | -      | linker                | UNP O66529 |
| ZB    | 46      | GLU      | -      | linker                | UNP O66529 |
| AC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| AC    | 37      | GLY      | -      | linker                | UNP O66529 |
| AC    | 38      | THR      | -      | linker                | UNP O66529 |
| AC    | 39      | GLY      | -      | linker                | UNP O66529 |
| AC    | 40      | GLY      | -      | linker                | UNP O66529 |
| AC    | 41      | SER      | -      | linker                | UNP O66529 |
| AC    | 42      | GLY      | -      | linker                | UNP O66529 |
| AC    | 43      | SER      | -      | linker                | UNP O66529 |
| AC    | 44      | SER      | -      | linker                | UNP O66529 |
| AC    | 45      | MET      | -      | linker                | UNP O66529 |
| AC    | 46      | GLU      | -      | linker                | UNP O66529 |
| BC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| BC    | 37      | GLY      | -      | linker                | UNP O66529 |
| BC    | 38      | THR      | -      | linker                | UNP O66529 |
| BC    | 39      | GLY      | -      | linker                | UNP O66529 |
| BC    | 40      | GLY      | -      | linker                | UNP O66529 |
| BC    | 41      | SER      | -      | linker                | UNP O66529 |
| BC    | 42      | GLY      | -      | linker                | UNP O66529 |
| BC    | 43      | SER      | -      | linker                | UNP O66529 |
| BC    | 44      | SER      | -      | linker                | UNP O66529 |
| BC    | 45      | MET      | -      | linker                | UNP O66529 |
| BC    | 46      | GLU      | -      | linker                | UNP O66529 |
| CC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| CC    | 37      | GLY      | -      | linker                | UNP O66529 |
| CC    | 38      | THR      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CC    | 39      | GLY      | -      | linker                | UNP O66529 |
| CC    | 40      | GLY      | -      | linker                | UNP O66529 |
| CC    | 41      | SER      | -      | linker                | UNP O66529 |
| CC    | 42      | GLY      | -      | linker                | UNP O66529 |
| CC    | 43      | SER      | -      | linker                | UNP O66529 |
| CC    | 44      | SER      | -      | linker                | UNP O66529 |
| CC    | 45      | MET      | -      | linker                | UNP O66529 |
| CC    | 46      | GLU      | -      | linker                | UNP O66529 |
| DC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| DC    | 37      | GLY      | -      | linker                | UNP O66529 |
| DC    | 38      | THR      | -      | linker                | UNP O66529 |
| DC    | 39      | GLY      | -      | linker                | UNP O66529 |
| DC    | 40      | GLY      | -      | linker                | UNP O66529 |
| DC    | 41      | SER      | -      | linker                | UNP O66529 |
| DC    | 42      | GLY      | -      | linker                | UNP O66529 |
| DC    | 43      | SER      | -      | linker                | UNP O66529 |
| DC    | 44      | SER      | -      | linker                | UNP O66529 |
| DC    | 45      | MET      | -      | linker                | UNP O66529 |
| DC    | 46      | GLU      | -      | linker                | UNP O66529 |
| EC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| EC    | 37      | GLY      | -      | linker                | UNP O66529 |
| EC    | 38      | THR      | -      | linker                | UNP O66529 |
| EC    | 39      | GLY      | -      | linker                | UNP O66529 |
| EC    | 40      | GLY      | -      | linker                | UNP O66529 |
| EC    | 41      | SER      | -      | linker                | UNP O66529 |
| EC    | 42      | GLY      | -      | linker                | UNP O66529 |
| EC    | 43      | SER      | -      | linker                | UNP O66529 |
| EC    | 44      | SER      | -      | linker                | UNP O66529 |
| EC    | 45      | MET      | -      | linker                | UNP O66529 |
| EC    | 46      | GLU      | -      | linker                | UNP O66529 |
| FC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| FC    | 37      | GLY      | -      | linker                | UNP O66529 |
| FC    | 38      | THR      | -      | linker                | UNP O66529 |
| FC    | 39      | GLY      | -      | linker                | UNP O66529 |
| FC    | 40      | GLY      | -      | linker                | UNP O66529 |
| FC    | 41      | SER      | -      | linker                | UNP O66529 |
| FC    | 42      | GLY      | -      | linker                | UNP O66529 |
| FC    | 43      | SER      | -      | linker                | UNP O66529 |
| FC    | 44      | SER      | -      | linker                | UNP O66529 |
| FC    | 45      | MET      | -      | linker                | UNP O66529 |
| FC    | 46      | GLU      | -      | linker                | UNP O66529 |
| GC    | 1       | MET      | -      | initiating methionine | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| GC    | 37      | GLY      | -      | linker                | UNP O66529 |
| GC    | 38      | THR      | -      | linker                | UNP O66529 |
| GC    | 39      | GLY      | -      | linker                | UNP O66529 |
| GC    | 40      | GLY      | -      | linker                | UNP O66529 |
| GC    | 41      | SER      | -      | linker                | UNP O66529 |
| GC    | 42      | GLY      | -      | linker                | UNP O66529 |
| GC    | 43      | SER      | -      | linker                | UNP O66529 |
| GC    | 44      | SER      | -      | linker                | UNP O66529 |
| GC    | 45      | MET      | -      | linker                | UNP O66529 |
| GC    | 46      | GLU      | -      | linker                | UNP O66529 |
| HC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| HC    | 37      | GLY      | -      | linker                | UNP O66529 |
| HC    | 38      | THR      | -      | linker                | UNP O66529 |
| HC    | 39      | GLY      | -      | linker                | UNP O66529 |
| HC    | 40      | GLY      | -      | linker                | UNP O66529 |
| HC    | 41      | SER      | -      | linker                | UNP O66529 |
| HC    | 42      | GLY      | -      | linker                | UNP O66529 |
| HC    | 43      | SER      | -      | linker                | UNP O66529 |
| HC    | 44      | SER      | -      | linker                | UNP O66529 |
| HC    | 45      | MET      | -      | linker                | UNP O66529 |
| HC    | 46      | GLU      | -      | linker                | UNP O66529 |
| IC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| IC    | 37      | GLY      | -      | linker                | UNP O66529 |
| IC    | 38      | THR      | -      | linker                | UNP O66529 |
| IC    | 39      | GLY      | -      | linker                | UNP O66529 |
| IC    | 40      | GLY      | -      | linker                | UNP O66529 |
| IC    | 41      | SER      | -      | linker                | UNP O66529 |
| IC    | 42      | GLY      | -      | linker                | UNP O66529 |
| IC    | 43      | SER      | -      | linker                | UNP O66529 |
| IC    | 44      | SER      | -      | linker                | UNP O66529 |
| IC    | 45      | MET      | -      | linker                | UNP O66529 |
| IC    | 46      | GLU      | -      | linker                | UNP O66529 |
| JC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| JC    | 37      | GLY      | -      | linker                | UNP O66529 |
| JC    | 38      | THR      | -      | linker                | UNP O66529 |
| JC    | 39      | GLY      | -      | linker                | UNP O66529 |
| JC    | 40      | GLY      | -      | linker                | UNP O66529 |
| JC    | 41      | SER      | -      | linker                | UNP O66529 |
| JC    | 42      | GLY      | -      | linker                | UNP O66529 |
| JC    | 43      | SER      | -      | linker                | UNP O66529 |
| JC    | 44      | SER      | -      | linker                | UNP O66529 |
| JC    | 45      | MET      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| JC    | 46      | GLU      | -      | linker                | UNP O66529 |
| KC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| KC    | 37      | GLY      | -      | linker                | UNP O66529 |
| KC    | 38      | THR      | -      | linker                | UNP O66529 |
| KC    | 39      | GLY      | -      | linker                | UNP O66529 |
| KC    | 40      | GLY      | -      | linker                | UNP O66529 |
| KC    | 41      | SER      | -      | linker                | UNP O66529 |
| KC    | 42      | GLY      | -      | linker                | UNP O66529 |
| KC    | 43      | SER      | -      | linker                | UNP O66529 |
| KC    | 44      | SER      | -      | linker                | UNP O66529 |
| KC    | 45      | MET      | -      | linker                | UNP O66529 |
| KC    | 46      | GLU      | -      | linker                | UNP O66529 |
| LC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| LC    | 37      | GLY      | -      | linker                | UNP O66529 |
| LC    | 38      | THR      | -      | linker                | UNP O66529 |
| LC    | 39      | GLY      | -      | linker                | UNP O66529 |
| LC    | 40      | GLY      | -      | linker                | UNP O66529 |
| LC    | 41      | SER      | -      | linker                | UNP O66529 |
| LC    | 42      | GLY      | -      | linker                | UNP O66529 |
| LC    | 43      | SER      | -      | linker                | UNP O66529 |
| LC    | 44      | SER      | -      | linker                | UNP O66529 |
| LC    | 45      | MET      | -      | linker                | UNP O66529 |
| LC    | 46      | GLU      | -      | linker                | UNP O66529 |
| MC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| MC    | 37      | GLY      | -      | linker                | UNP O66529 |
| MC    | 38      | THR      | -      | linker                | UNP O66529 |
| MC    | 39      | GLY      | -      | linker                | UNP O66529 |
| MC    | 40      | GLY      | -      | linker                | UNP O66529 |
| MC    | 41      | SER      | -      | linker                | UNP O66529 |
| MC    | 42      | GLY      | -      | linker                | UNP O66529 |
| MC    | 43      | SER      | -      | linker                | UNP O66529 |
| MC    | 44      | SER      | -      | linker                | UNP O66529 |
| MC    | 45      | MET      | -      | linker                | UNP O66529 |
| MC    | 46      | GLU      | -      | linker                | UNP O66529 |
| NC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| NC    | 37      | GLY      | -      | linker                | UNP O66529 |
| NC    | 38      | THR      | -      | linker                | UNP O66529 |
| NC    | 39      | GLY      | -      | linker                | UNP O66529 |
| NC    | 40      | GLY      | -      | linker                | UNP O66529 |
| NC    | 41      | SER      | -      | linker                | UNP O66529 |
| NC    | 42      | GLY      | -      | linker                | UNP O66529 |
| NC    | 43      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| NC    | 44      | SER      | -      | linker                | UNP O66529 |
| NC    | 45      | MET      | -      | linker                | UNP O66529 |
| NC    | 46      | GLU      | -      | linker                | UNP O66529 |
| OC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| OC    | 37      | GLY      | -      | linker                | UNP O66529 |
| OC    | 38      | THR      | -      | linker                | UNP O66529 |
| OC    | 39      | GLY      | -      | linker                | UNP O66529 |
| OC    | 40      | GLY      | -      | linker                | UNP O66529 |
| OC    | 41      | SER      | -      | linker                | UNP O66529 |
| OC    | 42      | GLY      | -      | linker                | UNP O66529 |
| OC    | 43      | SER      | -      | linker                | UNP O66529 |
| OC    | 44      | SER      | -      | linker                | UNP O66529 |
| OC    | 45      | MET      | -      | linker                | UNP O66529 |
| OC    | 46      | GLU      | -      | linker                | UNP O66529 |
| PC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| PC    | 37      | GLY      | -      | linker                | UNP O66529 |
| PC    | 38      | THR      | -      | linker                | UNP O66529 |
| PC    | 39      | GLY      | -      | linker                | UNP O66529 |
| PC    | 40      | GLY      | -      | linker                | UNP O66529 |
| PC    | 41      | SER      | -      | linker                | UNP O66529 |
| PC    | 42      | GLY      | -      | linker                | UNP O66529 |
| PC    | 43      | SER      | -      | linker                | UNP O66529 |
| PC    | 44      | SER      | -      | linker                | UNP O66529 |
| PC    | 45      | MET      | -      | linker                | UNP O66529 |
| PC    | 46      | GLU      | -      | linker                | UNP O66529 |
| QC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| QC    | 37      | GLY      | -      | linker                | UNP O66529 |
| QC    | 38      | THR      | -      | linker                | UNP O66529 |
| QC    | 39      | GLY      | -      | linker                | UNP O66529 |
| QC    | 40      | GLY      | -      | linker                | UNP O66529 |
| QC    | 41      | SER      | -      | linker                | UNP O66529 |
| QC    | 42      | GLY      | -      | linker                | UNP O66529 |
| QC    | 43      | SER      | -      | linker                | UNP O66529 |
| QC    | 44      | SER      | -      | linker                | UNP O66529 |
| QC    | 45      | MET      | -      | linker                | UNP O66529 |
| QC    | 46      | GLU      | -      | linker                | UNP O66529 |
| RC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| RC    | 37      | GLY      | -      | linker                | UNP O66529 |
| RC    | 38      | THR      | -      | linker                | UNP O66529 |
| RC    | 39      | GLY      | -      | linker                | UNP O66529 |
| RC    | 40      | GLY      | -      | linker                | UNP O66529 |
| RC    | 41      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| RC    | 42      | GLY      | -      | linker                | UNP O66529 |
| RC    | 43      | SER      | -      | linker                | UNP O66529 |
| RC    | 44      | SER      | -      | linker                | UNP O66529 |
| RC    | 45      | MET      | -      | linker                | UNP O66529 |
| RC    | 46      | GLU      | -      | linker                | UNP O66529 |
| SC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| SC    | 37      | GLY      | -      | linker                | UNP O66529 |
| SC    | 38      | THR      | -      | linker                | UNP O66529 |
| SC    | 39      | GLY      | -      | linker                | UNP O66529 |
| SC    | 40      | GLY      | -      | linker                | UNP O66529 |
| SC    | 41      | SER      | -      | linker                | UNP O66529 |
| SC    | 42      | GLY      | -      | linker                | UNP O66529 |
| SC    | 43      | SER      | -      | linker                | UNP O66529 |
| SC    | 44      | SER      | -      | linker                | UNP O66529 |
| SC    | 45      | MET      | -      | linker                | UNP O66529 |
| SC    | 46      | GLU      | -      | linker                | UNP O66529 |
| TC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| TC    | 37      | GLY      | -      | linker                | UNP O66529 |
| TC    | 38      | THR      | -      | linker                | UNP O66529 |
| TC    | 39      | GLY      | -      | linker                | UNP O66529 |
| TC    | 40      | GLY      | -      | linker                | UNP O66529 |
| TC    | 41      | SER      | -      | linker                | UNP O66529 |
| TC    | 42      | GLY      | -      | linker                | UNP O66529 |
| TC    | 43      | SER      | -      | linker                | UNP O66529 |
| TC    | 44      | SER      | -      | linker                | UNP O66529 |
| TC    | 45      | MET      | -      | linker                | UNP O66529 |
| TC    | 46      | GLU      | -      | linker                | UNP O66529 |
| UC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| UC    | 37      | GLY      | -      | linker                | UNP O66529 |
| UC    | 38      | THR      | -      | linker                | UNP O66529 |
| UC    | 39      | GLY      | -      | linker                | UNP O66529 |
| UC    | 40      | GLY      | -      | linker                | UNP O66529 |
| UC    | 41      | SER      | -      | linker                | UNP O66529 |
| UC    | 42      | GLY      | -      | linker                | UNP O66529 |
| UC    | 43      | SER      | -      | linker                | UNP O66529 |
| UC    | 44      | SER      | -      | linker                | UNP O66529 |
| UC    | 45      | MET      | -      | linker                | UNP O66529 |
| UC    | 46      | GLU      | -      | linker                | UNP O66529 |
| VC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| VC    | 37      | GLY      | -      | linker                | UNP O66529 |
| VC    | 38      | THR      | -      | linker                | UNP O66529 |
| VC    | 39      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| VC    | 40      | GLY      | -      | linker                | UNP O66529 |
| VC    | 41      | SER      | -      | linker                | UNP O66529 |
| VC    | 42      | GLY      | -      | linker                | UNP O66529 |
| VC    | 43      | SER      | -      | linker                | UNP O66529 |
| VC    | 44      | SER      | -      | linker                | UNP O66529 |
| VC    | 45      | MET      | -      | linker                | UNP O66529 |
| VC    | 46      | GLU      | -      | linker                | UNP O66529 |
| WC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| WC    | 37      | GLY      | -      | linker                | UNP O66529 |
| WC    | 38      | THR      | -      | linker                | UNP O66529 |
| WC    | 39      | GLY      | -      | linker                | UNP O66529 |
| WC    | 40      | GLY      | -      | linker                | UNP O66529 |
| WC    | 41      | SER      | -      | linker                | UNP O66529 |
| WC    | 42      | GLY      | -      | linker                | UNP O66529 |
| WC    | 43      | SER      | -      | linker                | UNP O66529 |
| WC    | 44      | SER      | -      | linker                | UNP O66529 |
| WC    | 45      | MET      | -      | linker                | UNP O66529 |
| WC    | 46      | GLU      | -      | linker                | UNP O66529 |
| XC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| XC    | 37      | GLY      | -      | linker                | UNP O66529 |
| XC    | 38      | THR      | -      | linker                | UNP O66529 |
| XC    | 39      | GLY      | -      | linker                | UNP O66529 |
| XC    | 40      | GLY      | -      | linker                | UNP O66529 |
| XC    | 41      | SER      | -      | linker                | UNP O66529 |
| XC    | 42      | GLY      | -      | linker                | UNP O66529 |
| XC    | 43      | SER      | -      | linker                | UNP O66529 |
| XC    | 44      | SER      | -      | linker                | UNP O66529 |
| XC    | 45      | MET      | -      | linker                | UNP O66529 |
| XC    | 46      | GLU      | -      | linker                | UNP O66529 |
| YC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| YC    | 37      | GLY      | -      | linker                | UNP O66529 |
| YC    | 38      | THR      | -      | linker                | UNP O66529 |
| YC    | 39      | GLY      | -      | linker                | UNP O66529 |
| YC    | 40      | GLY      | -      | linker                | UNP O66529 |
| YC    | 41      | SER      | -      | linker                | UNP O66529 |
| YC    | 42      | GLY      | -      | linker                | UNP O66529 |
| YC    | 43      | SER      | -      | linker                | UNP O66529 |
| YC    | 44      | SER      | -      | linker                | UNP O66529 |
| YC    | 45      | MET      | -      | linker                | UNP O66529 |
| YC    | 46      | GLU      | -      | linker                | UNP O66529 |
| ZC    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| ZC    | 37      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| ZC    | 38      | THR      | -      | linker                | UNP O66529 |
| ZC    | 39      | GLY      | -      | linker                | UNP O66529 |
| ZC    | 40      | GLY      | -      | linker                | UNP O66529 |
| ZC    | 41      | SER      | -      | linker                | UNP O66529 |
| ZC    | 42      | GLY      | -      | linker                | UNP O66529 |
| ZC    | 43      | SER      | -      | linker                | UNP O66529 |
| ZC    | 44      | SER      | -      | linker                | UNP O66529 |
| ZC    | 45      | MET      | -      | linker                | UNP O66529 |
| ZC    | 46      | GLU      | -      | linker                | UNP O66529 |
| AD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| AD    | 37      | GLY      | -      | linker                | UNP O66529 |
| AD    | 38      | THR      | -      | linker                | UNP O66529 |
| AD    | 39      | GLY      | -      | linker                | UNP O66529 |
| AD    | 40      | GLY      | -      | linker                | UNP O66529 |
| AD    | 41      | SER      | -      | linker                | UNP O66529 |
| AD    | 42      | GLY      | -      | linker                | UNP O66529 |
| AD    | 43      | SER      | -      | linker                | UNP O66529 |
| AD    | 44      | SER      | -      | linker                | UNP O66529 |
| AD    | 45      | MET      | -      | linker                | UNP O66529 |
| AD    | 46      | GLU      | -      | linker                | UNP O66529 |
| BD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| BD    | 37      | GLY      | -      | linker                | UNP O66529 |
| BD    | 38      | THR      | -      | linker                | UNP O66529 |
| BD    | 39      | GLY      | -      | linker                | UNP O66529 |
| BD    | 40      | GLY      | -      | linker                | UNP O66529 |
| BD    | 41      | SER      | -      | linker                | UNP O66529 |
| BD    | 42      | GLY      | -      | linker                | UNP O66529 |
| BD    | 43      | SER      | -      | linker                | UNP O66529 |
| BD    | 44      | SER      | -      | linker                | UNP O66529 |
| BD    | 45      | MET      | -      | linker                | UNP O66529 |
| BD    | 46      | GLU      | -      | linker                | UNP O66529 |
| CD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| CD    | 37      | GLY      | -      | linker                | UNP O66529 |
| CD    | 38      | THR      | -      | linker                | UNP O66529 |
| CD    | 39      | GLY      | -      | linker                | UNP O66529 |
| CD    | 40      | GLY      | -      | linker                | UNP O66529 |
| CD    | 41      | SER      | -      | linker                | UNP O66529 |
| CD    | 42      | GLY      | -      | linker                | UNP O66529 |
| CD    | 43      | SER      | -      | linker                | UNP O66529 |
| CD    | 44      | SER      | -      | linker                | UNP O66529 |
| CD    | 45      | MET      | -      | linker                | UNP O66529 |
| CD    | 46      | GLU      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| DD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| DD    | 37      | GLY      | -      | linker                | UNP O66529 |
| DD    | 38      | THR      | -      | linker                | UNP O66529 |
| DD    | 39      | GLY      | -      | linker                | UNP O66529 |
| DD    | 40      | GLY      | -      | linker                | UNP O66529 |
| DD    | 41      | SER      | -      | linker                | UNP O66529 |
| DD    | 42      | GLY      | -      | linker                | UNP O66529 |
| DD    | 43      | SER      | -      | linker                | UNP O66529 |
| DD    | 44      | SER      | -      | linker                | UNP O66529 |
| DD    | 45      | MET      | -      | linker                | UNP O66529 |
| DD    | 46      | GLU      | -      | linker                | UNP O66529 |
| ED    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| ED    | 37      | GLY      | -      | linker                | UNP O66529 |
| ED    | 38      | THR      | -      | linker                | UNP O66529 |
| ED    | 39      | GLY      | -      | linker                | UNP O66529 |
| ED    | 40      | GLY      | -      | linker                | UNP O66529 |
| ED    | 41      | SER      | -      | linker                | UNP O66529 |
| ED    | 42      | GLY      | -      | linker                | UNP O66529 |
| ED    | 43      | SER      | -      | linker                | UNP O66529 |
| ED    | 44      | SER      | -      | linker                | UNP O66529 |
| ED    | 45      | MET      | -      | linker                | UNP O66529 |
| ED    | 46      | GLU      | -      | linker                | UNP O66529 |
| FD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| FD    | 37      | GLY      | -      | linker                | UNP O66529 |
| FD    | 38      | THR      | -      | linker                | UNP O66529 |
| FD    | 39      | GLY      | -      | linker                | UNP O66529 |
| FD    | 40      | GLY      | -      | linker                | UNP O66529 |
| FD    | 41      | SER      | -      | linker                | UNP O66529 |
| FD    | 42      | GLY      | -      | linker                | UNP O66529 |
| FD    | 43      | SER      | -      | linker                | UNP O66529 |
| FD    | 44      | SER      | -      | linker                | UNP O66529 |
| FD    | 45      | MET      | -      | linker                | UNP O66529 |
| FD    | 46      | GLU      | -      | linker                | UNP O66529 |
| GD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| GD    | 37      | GLY      | -      | linker                | UNP O66529 |
| GD    | 38      | THR      | -      | linker                | UNP O66529 |
| GD    | 39      | GLY      | -      | linker                | UNP O66529 |
| GD    | 40      | GLY      | -      | linker                | UNP O66529 |
| GD    | 41      | SER      | -      | linker                | UNP O66529 |
| GD    | 42      | GLY      | -      | linker                | UNP O66529 |
| GD    | 43      | SER      | -      | linker                | UNP O66529 |
| GD    | 44      | SER      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| GD    | 45      | MET      | -      | linker                | UNP O66529 |
| GD    | 46      | GLU      | -      | linker                | UNP O66529 |
| HD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| HD    | 37      | GLY      | -      | linker                | UNP O66529 |
| HD    | 38      | THR      | -      | linker                | UNP O66529 |
| HD    | 39      | GLY      | -      | linker                | UNP O66529 |
| HD    | 40      | GLY      | -      | linker                | UNP O66529 |
| HD    | 41      | SER      | -      | linker                | UNP O66529 |
| HD    | 42      | GLY      | -      | linker                | UNP O66529 |
| HD    | 43      | SER      | -      | linker                | UNP O66529 |
| HD    | 44      | SER      | -      | linker                | UNP O66529 |
| HD    | 45      | MET      | -      | linker                | UNP O66529 |
| HD    | 46      | GLU      | -      | linker                | UNP O66529 |
| ID    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| ID    | 37      | GLY      | -      | linker                | UNP O66529 |
| ID    | 38      | THR      | -      | linker                | UNP O66529 |
| ID    | 39      | GLY      | -      | linker                | UNP O66529 |
| ID    | 40      | GLY      | -      | linker                | UNP O66529 |
| ID    | 41      | SER      | -      | linker                | UNP O66529 |
| ID    | 42      | GLY      | -      | linker                | UNP O66529 |
| ID    | 43      | SER      | -      | linker                | UNP O66529 |
| ID    | 44      | SER      | -      | linker                | UNP O66529 |
| ID    | 45      | MET      | -      | linker                | UNP O66529 |
| ID    | 46      | GLU      | -      | linker                | UNP O66529 |
| JD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| JD    | 37      | GLY      | -      | linker                | UNP O66529 |
| JD    | 38      | THR      | -      | linker                | UNP O66529 |
| JD    | 39      | GLY      | -      | linker                | UNP O66529 |
| JD    | 40      | GLY      | -      | linker                | UNP O66529 |
| JD    | 41      | SER      | -      | linker                | UNP O66529 |
| JD    | 42      | GLY      | -      | linker                | UNP O66529 |
| JD    | 43      | SER      | -      | linker                | UNP O66529 |
| JD    | 44      | SER      | -      | linker                | UNP O66529 |
| JD    | 45      | MET      | -      | linker                | UNP O66529 |
| JD    | 46      | GLU      | -      | linker                | UNP O66529 |
| KD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| KD    | 37      | GLY      | -      | linker                | UNP O66529 |
| KD    | 38      | THR      | -      | linker                | UNP O66529 |
| KD    | 39      | GLY      | -      | linker                | UNP O66529 |
| KD    | 40      | GLY      | -      | linker                | UNP O66529 |
| KD    | 41      | SER      | -      | linker                | UNP O66529 |
| KD    | 42      | GLY      | -      | linker                | UNP O66529 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| KD    | 43      | SER      | -      | linker                | UNP O66529 |
| KD    | 44      | SER      | -      | linker                | UNP O66529 |
| KD    | 45      | MET      | -      | linker                | UNP O66529 |
| KD    | 46      | GLU      | -      | linker                | UNP O66529 |
| LD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| LD    | 37      | GLY      | -      | linker                | UNP O66529 |
| LD    | 38      | THR      | -      | linker                | UNP O66529 |
| LD    | 39      | GLY      | -      | linker                | UNP O66529 |
| LD    | 40      | GLY      | -      | linker                | UNP O66529 |
| LD    | 41      | SER      | -      | linker                | UNP O66529 |
| LD    | 42      | GLY      | -      | linker                | UNP O66529 |
| LD    | 43      | SER      | -      | linker                | UNP O66529 |
| LD    | 44      | SER      | -      | linker                | UNP O66529 |
| LD    | 45      | MET      | -      | linker                | UNP O66529 |
| LD    | 46      | GLU      | -      | linker                | UNP O66529 |
| MD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| MD    | 37      | GLY      | -      | linker                | UNP O66529 |
| MD    | 38      | THR      | -      | linker                | UNP O66529 |
| MD    | 39      | GLY      | -      | linker                | UNP O66529 |
| MD    | 40      | GLY      | -      | linker                | UNP O66529 |
| MD    | 41      | SER      | -      | linker                | UNP O66529 |
| MD    | 42      | GLY      | -      | linker                | UNP O66529 |
| MD    | 43      | SER      | -      | linker                | UNP O66529 |
| MD    | 44      | SER      | -      | linker                | UNP O66529 |
| MD    | 45      | MET      | -      | linker                | UNP O66529 |
| MD    | 46      | GLU      | -      | linker                | UNP O66529 |
| ND    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| ND    | 37      | GLY      | -      | linker                | UNP O66529 |
| ND    | 38      | THR      | -      | linker                | UNP O66529 |
| ND    | 39      | GLY      | -      | linker                | UNP O66529 |
| ND    | 40      | GLY      | -      | linker                | UNP O66529 |
| ND    | 41      | SER      | -      | linker                | UNP O66529 |
| ND    | 42      | GLY      | -      | linker                | UNP O66529 |
| ND    | 43      | SER      | -      | linker                | UNP O66529 |
| ND    | 44      | SER      | -      | linker                | UNP O66529 |
| ND    | 45      | MET      | -      | linker                | UNP O66529 |
| ND    | 46      | GLU      | -      | linker                | UNP O66529 |
| OD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| OD    | 37      | GLY      | -      | linker                | UNP O66529 |
| OD    | 38      | THR      | -      | linker                | UNP O66529 |
| OD    | 39      | GLY      | -      | linker                | UNP O66529 |
| OD    | 40      | GLY      | -      | linker                | UNP O66529 |

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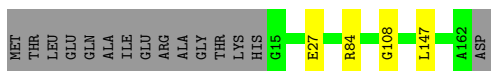
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| OD    | 41      | SER      | -      | linker                | UNP O66529 |
| OD    | 42      | GLY      | -      | linker                | UNP O66529 |
| OD    | 43      | SER      | -      | linker                | UNP O66529 |
| OD    | 44      | SER      | -      | linker                | UNP O66529 |
| OD    | 45      | MET      | -      | linker                | UNP O66529 |
| OD    | 46      | GLU      | -      | linker                | UNP O66529 |
| PD    | 1       | MET      | -      | initiating methionine | UNP O66529 |
| PD    | 37      | GLY      | -      | linker                | UNP O66529 |
| PD    | 38      | THR      | -      | linker                | UNP O66529 |
| PD    | 39      | GLY      | -      | linker                | UNP O66529 |
| PD    | 40      | GLY      | -      | linker                | UNP O66529 |
| PD    | 41      | SER      | -      | linker                | UNP O66529 |
| PD    | 42      | GLY      | -      | linker                | UNP O66529 |
| PD    | 43      | SER      | -      | linker                | UNP O66529 |
| PD    | 44      | SER      | -      | linker                | UNP O66529 |
| PD    | 45      | MET      | -      | linker                | UNP O66529 |
| PD    | 46      | GLU      | -      | linker                | UNP O66529 |

### 3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 6,7-dimethyl-8-ribityllumazine synthase

Chain A:  88% 9%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B:  88% 9%



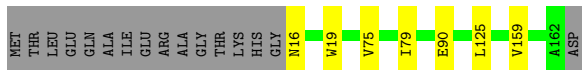
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C:  87% 9%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain D:  86% 10%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain E:  88% 5% 7%



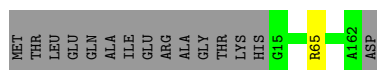
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F:  83% 7% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain G: 90% 9%



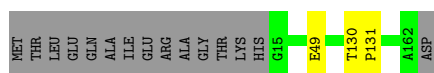
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain H: 91% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain I: 89% 9%



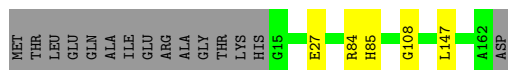
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J: 88% 8%



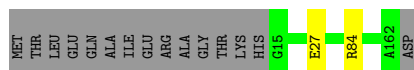
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain K: 88% 9%



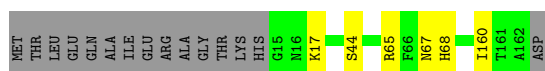
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain L: 90% 9%



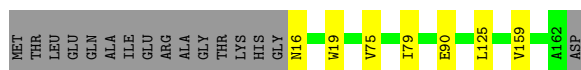
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain M: 87% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain N: 86% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain O: 88% 5% 7%



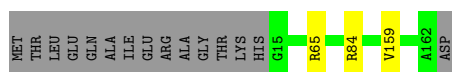
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain P: 83% 7% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Q: 89% 9%



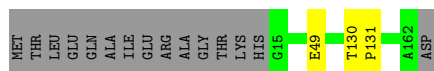
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain R: 90% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

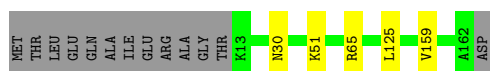
Chain S: 89% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

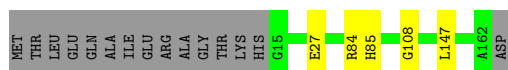
Chain T: 89% 8%





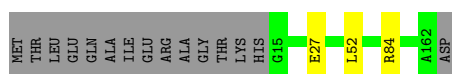
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain U: 88% 9%



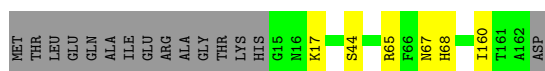
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain V: 89% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain W: 87% 9%



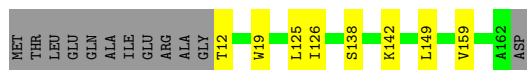
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain X: 86% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Y: 88% 5% 7%



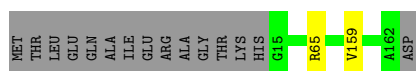
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Z: 83% 7% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AA: 90% 9%



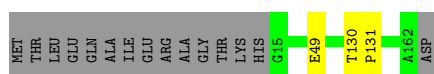
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BA: 90% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CA: 89% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DA: 87% 5% 8%



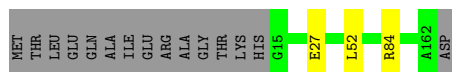
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EA: 88% 5% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FA: 89% 5% 9%



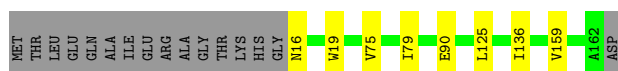
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GA: 87% 5% 9%



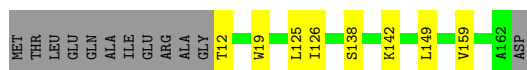
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HA: 85% 5% 10%



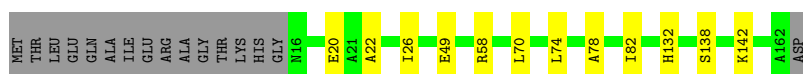
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IA: 88% 5% 7%



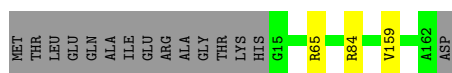
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JA: 83% 7% 10%



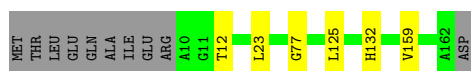
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KA: 89% 9% 2%



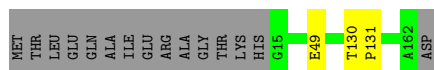
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LA: 90% 6% 4%



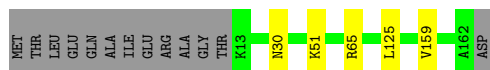
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MA: 89% 9% 2%



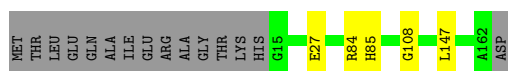
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NA: 89% 8% 3%

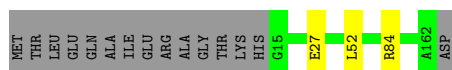


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

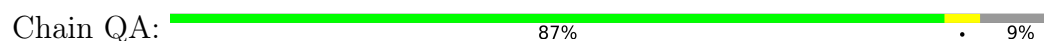
Chain OA: 88% 9% 3%



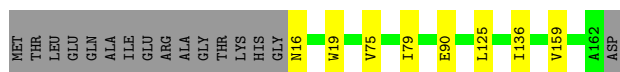
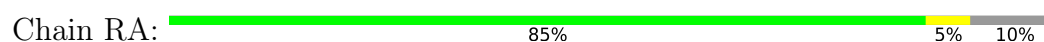
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



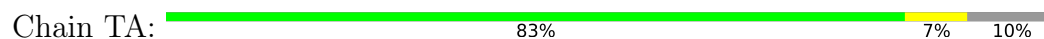
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



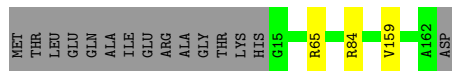
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



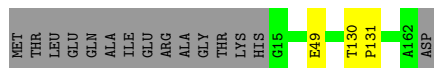
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase





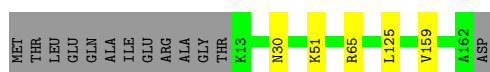
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WA: 89% 9%



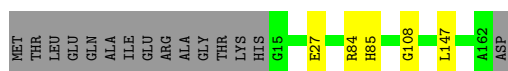
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XA: 89% 8%



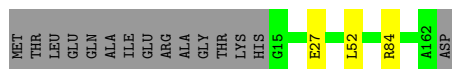
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YA: 88% 9%



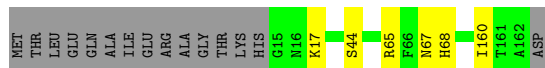
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZA: 89% 9%



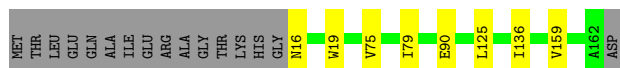
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AB: 87% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BB: 85% 5% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CB: 88% 5% 7%



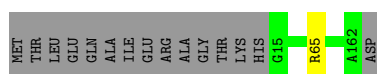
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DB: 83% 7% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EB: 90% 9%



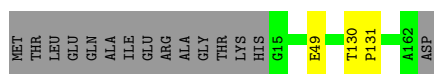
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FB: 91% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GB: 89% 9%



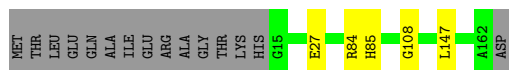
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HB: 88% 8%



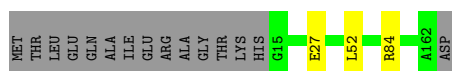
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IB: 88% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JB: 89% 9%



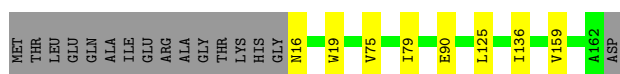
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KB: 87% 9%



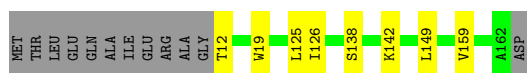
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LB: 85% 5% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MB: 88% 5% 7%



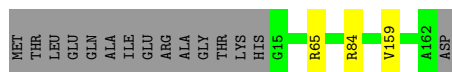
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NB: 83% 7% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OB: 89% 9% 2%



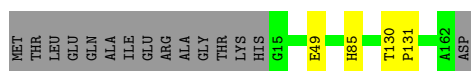
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PB: 90% 6% 4%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QB: 88% 9% 3%



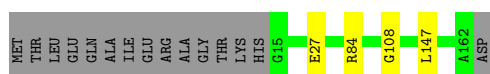
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RB: 88% 8%



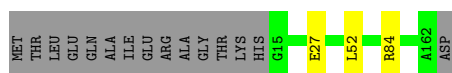
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SB: 88% 9%



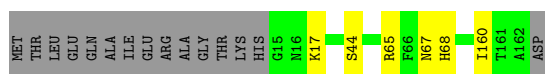
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TB: 89% 9%



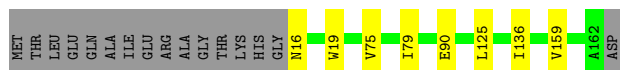
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UB: 87% 9%



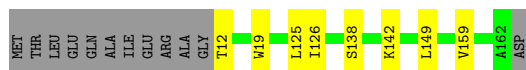
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VB: 85% 5% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WB: 88% 5% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

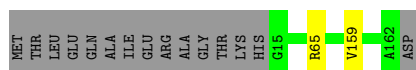
Chain XB: 83% 7% 10%





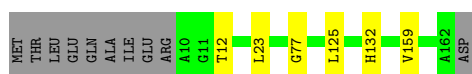
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YB: 90% 9%



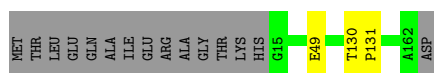
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZB: 90% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AC: 89% 9%



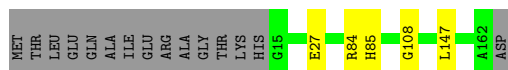
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BC: 88% 8%



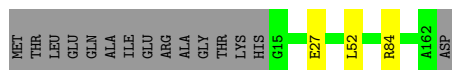
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CC: 88% 9%



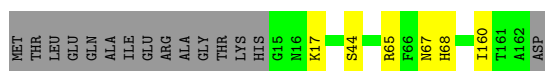
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DC: 89% 9%

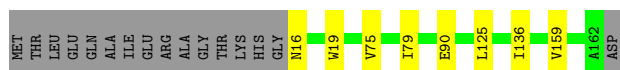
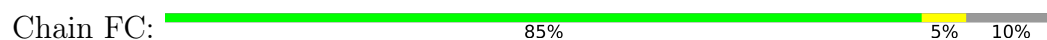


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EC: 87% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



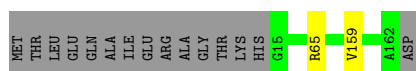
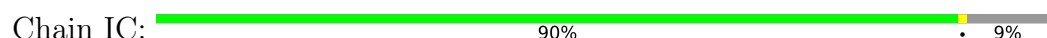
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



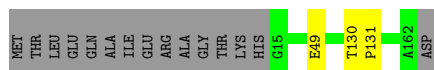
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

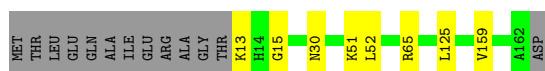


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



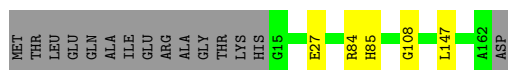
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase





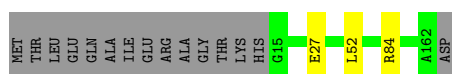
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MC: 88% 9%



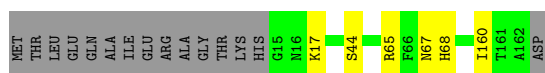
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NC: 89% 9%



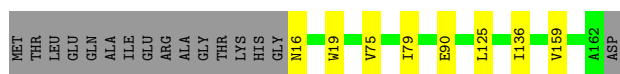
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OC: 87% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PC: 85% 5% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QC: 88% 5% 7%



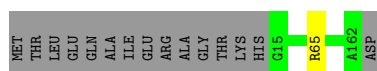
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RC: 83% 7% 10%



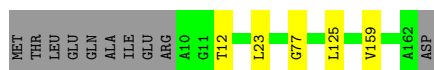
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SC: 90% 9%



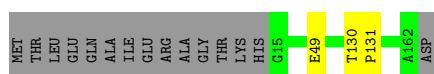
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TC: 91% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UC: 89% 9%



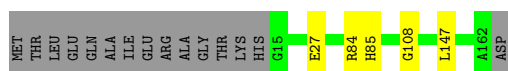
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VC: 88% 8%



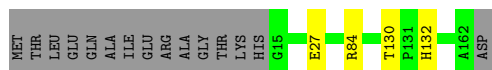
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WC: 88% 9%



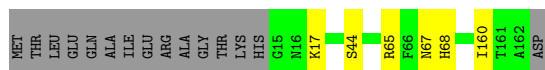
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XC: 88% 9%



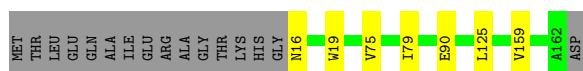
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YC: 87% 9%



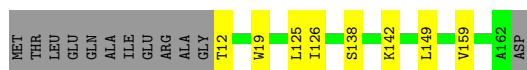
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZC: 86% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AD: 88% 5% 7%



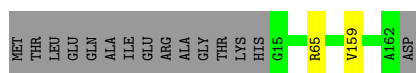
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BD: 83% 7% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CD: 90% • 9%



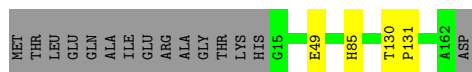
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DD: 90% • 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ED: 88% • 9%



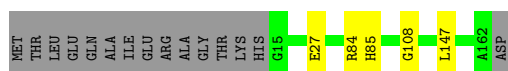
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FD: 88% • 8%



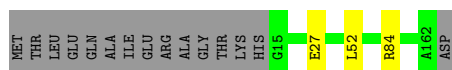
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GD: 88% • 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HD: 89% 9%



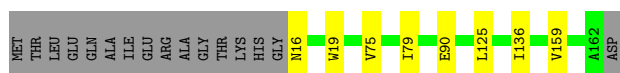
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ID: 87% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JD: 85% 5% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KD: 88% 5% 7%



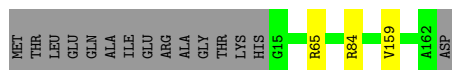
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LD: 83% 7% 10%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MD: 89% 9%

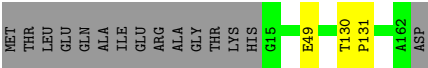
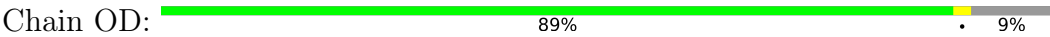


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

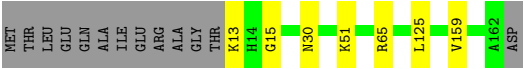
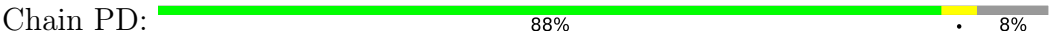
Chain ND: 90% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, T                                | Depositor |
| Number of particles used             | 83496                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 900                                     | Depositor |
| Maximum defocus (nm)                 | 2100                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K3 BIOCONTINUUM (6k x 4k)         | Depositor |



## 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     | 0.26         | 0/1125      | 0.52        | 0/1519      |
| 1   | AA    | 0.27         | 0/1125      | 0.52        | 0/1519      |
| 1   | AB    | 0.28         | 0/1125      | 0.54        | 0/1519      |
| 1   | AC    | 0.28         | 0/1125      | 0.52        | 0/1519      |
| 1   | AD    | 0.27         | 0/1152      | 0.53        | 0/1555      |
| 1   | B     | 0.27         | 0/1125      | 0.53        | 0/1519      |
| 1   | BA    | 0.29         | 0/1161      | 0.55        | 0/1567      |
| 1   | BB    | 0.26         | 0/1121      | 0.52        | 0/1514      |
| 1   | BC    | 0.27         | 0/1145      | 0.54        | 0/1545      |
| 1   | BD    | 0.26         | 0/1121      | 0.53        | 0/1514      |
| 1   | C     | 0.28         | 0/1125      | 0.54        | 0/1519      |
| 1   | CA    | 0.28         | 0/1125      | 0.52        | 0/1519      |
| 1   | CB    | 0.27         | 0/1152      | 0.53        | 0/1555      |
| 1   | CC    | 0.26         | 0/1125      | 0.52        | 0/1519      |
| 1   | CD    | 0.28         | 0/1125      | 0.52        | 0/1519      |
| 1   | D     | 0.26         | 0/1121      | 0.52        | 0/1514      |
| 1   | DA    | 0.27         | 0/1145      | 0.54        | 0/1545      |
| 1   | DB    | 0.26         | 0/1121      | 0.53        | 0/1514      |
| 1   | DC    | 0.27         | 0/1125      | 0.53        | 0/1519      |
| 1   | DD    | 0.29         | 0/1161      | 0.54        | 0/1567      |
| 1   | E     | 0.27         | 0/1152      | 0.53        | 0/1555      |
| 1   | EA    | 0.26         | 0/1125      | 0.52        | 0/1519      |
| 1   | EB    | 0.27         | 0/1125      | 0.53        | 0/1519      |
| 1   | EC    | 0.28         | 0/1125      | 0.54        | 0/1519      |
| 1   | ED    | 0.28         | 0/1125      | 0.52        | 0/1519      |
| 1   | F     | 0.26         | 0/1121      | 0.53        | 0/1514      |
| 1   | FA    | 0.27         | 0/1125      | 0.53        | 0/1519      |
| 1   | FB    | 0.29         | 0/1161      | 0.54        | 0/1567      |
| 1   | FC    | 0.26         | 0/1121      | 0.52        | 0/1514      |
| 1   | FD    | 0.27         | 0/1145      | 0.54        | 0/1545      |
| 1   | G     | 0.27         | 0/1125      | 0.52        | 0/1519      |
| 1   | GA    | 0.28         | 0/1125      | 0.54        | 0/1519      |
| 1   | GB    | 0.28         | 0/1125      | 0.52        | 0/1519      |
| 1   | GC    | 0.27         | 0/1152      | 0.53        | 0/1555      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | GD    | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | H     | 0.29         | 0/1161  | 0.54        | 0/1567  |
| 1   | HA    | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | HB    | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | HC    | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | HD    | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | I     | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | IA    | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | IB    | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | IC    | 0.27         | 0/1125  | 0.52        | 0/1519  |
| 1   | ID    | 0.28         | 0/1125  | 0.54        | 0/1519  |
| 1   | J     | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | JA    | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | JB    | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | JC    | 0.29         | 0/1161  | 0.54        | 0/1567  |
| 1   | JD    | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | K     | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | KA    | 0.28         | 0/1125  | 0.53        | 0/1519  |
| 1   | KB    | 0.27         | 0/1125  | 0.54        | 0/1519  |
| 1   | KC    | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | KD    | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | L     | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | LA    | 0.29         | 0/1161  | 0.55        | 0/1567  |
| 1   | LB    | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | LC    | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | LD    | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | M     | 0.28         | 0/1125  | 0.54        | 0/1519  |
| 1   | MA    | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | MB    | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | MC    | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | MD    | 0.27         | 0/1125  | 0.52        | 0/1519  |
| 1   | N     | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | NA    | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | NB    | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | NC    | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | ND    | 0.29         | 0/1161  | 0.54        | 0/1567  |
| 1   | O     | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | OA    | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | OB    | 0.27         | 0/1125  | 0.52        | 0/1519  |
| 1   | OC    | 0.28         | 0/1125  | 0.54        | 0/1519  |
| 1   | OD    | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | P     | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | PA    | 0.27         | 0/1125  | 0.53        | 0/1519  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | PB    | 0.29         | 0/1161  | 0.55        | 0/1567  |
| 1   | PC    | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | PD    | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | Q     | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | QA    | 0.28         | 0/1125  | 0.54        | 0/1519  |
| 1   | QB    | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | QC    | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | R     | 0.29         | 0/1161  | 0.55        | 0/1567  |
| 1   | RA    | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | RB    | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | RC    | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | S     | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | SA    | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | SB    | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | SC    | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | T     | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | TA    | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | TB    | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | TC    | 0.29         | 0/1161  | 0.55        | 0/1567  |
| 1   | U     | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | UA    | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | UB    | 0.28         | 0/1125  | 0.54        | 0/1519  |
| 1   | UC    | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | V     | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | VA    | 0.29         | 0/1161  | 0.54        | 0/1567  |
| 1   | VB    | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | VC    | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | W     | 0.28         | 0/1125  | 0.54        | 0/1519  |
| 1   | WA    | 0.28         | 0/1125  | 0.52        | 0/1519  |
| 1   | WB    | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | WC    | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | X     | 0.26         | 0/1121  | 0.52        | 0/1514  |
| 1   | XA    | 0.27         | 0/1145  | 0.54        | 0/1545  |
| 1   | XB    | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | XC    | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | Y     | 0.27         | 0/1152  | 0.53        | 0/1555  |
| 1   | YA    | 0.26         | 0/1125  | 0.52        | 0/1519  |
| 1   | YB    | 0.27         | 0/1125  | 0.52        | 0/1519  |
| 1   | YC    | 0.28         | 0/1125  | 0.54        | 0/1519  |
| 1   | Z     | 0.26         | 0/1121  | 0.53        | 0/1514  |
| 1   | ZA    | 0.27         | 0/1125  | 0.53        | 0/1519  |
| 1   | ZB    | 0.29         | 0/1161  | 0.54        | 0/1567  |
| 1   | ZC    | 0.26         | 0/1121  | 0.52        | 0/1514  |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| All | All   | 0.27         | 0/135900 | 0.53        | 0/183480 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1108  | 0        | 1126     | 7       | 0            |
| 1   | AA    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | AB    | 1108  | 0        | 1126     | 6       | 0            |
| 1   | AC    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | AD    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | B     | 1108  | 0        | 1126     | 5       | 0            |
| 1   | BA    | 1143  | 0        | 1161     | 5       | 0            |
| 1   | BB    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | BC    | 1127  | 0        | 1146     | 5       | 0            |
| 1   | BD    | 1104  | 0        | 1123     | 6       | 0            |
| 1   | C     | 1108  | 0        | 1126     | 7       | 0            |
| 1   | CA    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | CB    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | CC    | 1108  | 0        | 1126     | 8       | 0            |
| 1   | CD    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | D     | 1104  | 0        | 1123     | 5       | 0            |
| 1   | DA    | 1127  | 0        | 1146     | 6       | 0            |
| 1   | DB    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | DC    | 1108  | 0        | 1126     | 4       | 0            |
| 1   | DD    | 1143  | 0        | 1161     | 5       | 0            |
| 1   | E     | 1134  | 0        | 1153     | 6       | 0            |
| 1   | EA    | 1108  | 0        | 1126     | 8       | 0            |
| 1   | EB    | 1108  | 0        | 1126     | 1       | 0            |
| 1   | EC    | 1108  | 0        | 1126     | 6       | 0            |
| 1   | ED    | 1108  | 0        | 1126     | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | F     | 1104  | 0        | 1123     | 7       | 0            |
| 1   | FA    | 1108  | 0        | 1126     | 4       | 0            |
| 1   | FB    | 1143  | 0        | 1161     | 4       | 0            |
| 1   | FC    | 1104  | 0        | 1123     | 6       | 0            |
| 1   | FD    | 1127  | 0        | 1146     | 5       | 0            |
| 1   | G     | 1108  | 0        | 1126     | 1       | 0            |
| 1   | GA    | 1108  | 0        | 1126     | 7       | 0            |
| 1   | GB    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | GC    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | GD    | 1108  | 0        | 1126     | 8       | 0            |
| 1   | H     | 1143  | 0        | 1161     | 4       | 0            |
| 1   | HA    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | HB    | 1127  | 0        | 1146     | 5       | 0            |
| 1   | HC    | 1104  | 0        | 1123     | 6       | 0            |
| 1   | HD    | 1108  | 0        | 1126     | 4       | 0            |
| 1   | I     | 1108  | 0        | 1126     | 2       | 0            |
| 1   | IA    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | IB    | 1108  | 0        | 1126     | 8       | 0            |
| 1   | IC    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | ID    | 1108  | 0        | 1126     | 7       | 0            |
| 1   | J     | 1127  | 0        | 1146     | 5       | 0            |
| 1   | JA    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | JB    | 1108  | 0        | 1126     | 4       | 0            |
| 1   | JC    | 1143  | 0        | 1161     | 5       | 0            |
| 1   | JD    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | K     | 1108  | 0        | 1126     | 8       | 0            |
| 1   | KA    | 1108  | 0        | 1126     | 3       | 0            |
| 1   | KB    | 1108  | 0        | 1126     | 7       | 0            |
| 1   | KC    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | KD    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | L     | 1108  | 0        | 1126     | 3       | 0            |
| 1   | LA    | 1143  | 0        | 1161     | 5       | 0            |
| 1   | LB    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | LC    | 1127  | 0        | 1146     | 6       | 0            |
| 1   | LD    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | M     | 1108  | 0        | 1126     | 6       | 0            |
| 1   | MA    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | MB    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | MC    | 1108  | 0        | 1126     | 8       | 0            |
| 1   | MD    | 1108  | 0        | 1126     | 3       | 0            |
| 1   | N     | 1104  | 0        | 1123     | 6       | 0            |
| 1   | NA    | 1127  | 0        | 1146     | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | NB    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | NC    | 1108  | 0        | 1126     | 4       | 0            |
| 1   | ND    | 1143  | 0        | 1161     | 5       | 0            |
| 1   | O     | 1134  | 0        | 1153     | 6       | 0            |
| 1   | OA    | 1108  | 0        | 1126     | 8       | 0            |
| 1   | OB    | 1108  | 0        | 1126     | 3       | 0            |
| 1   | OC    | 1108  | 0        | 1126     | 6       | 0            |
| 1   | OD    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | P     | 1104  | 0        | 1123     | 6       | 0            |
| 1   | PA    | 1108  | 0        | 1126     | 4       | 0            |
| 1   | PB    | 1143  | 0        | 1161     | 5       | 0            |
| 1   | PC    | 1104  | 0        | 1123     | 6       | 0            |
| 1   | PD    | 1127  | 0        | 1146     | 5       | 0            |
| 1   | Q     | 1108  | 0        | 1126     | 3       | 0            |
| 1   | QA    | 1108  | 0        | 1126     | 7       | 0            |
| 1   | QB    | 1108  | 0        | 1126     | 3       | 0            |
| 1   | QC    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | R     | 1143  | 0        | 1161     | 5       | 0            |
| 1   | RA    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | RB    | 1127  | 0        | 1146     | 5       | 0            |
| 1   | RC    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | S     | 1108  | 0        | 1126     | 2       | 0            |
| 1   | SA    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | SB    | 1108  | 0        | 1126     | 7       | 0            |
| 1   | SC    | 1108  | 0        | 1126     | 1       | 0            |
| 1   | T     | 1127  | 0        | 1146     | 4       | 0            |
| 1   | TA    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | TB    | 1108  | 0        | 1126     | 4       | 0            |
| 1   | TC    | 1143  | 0        | 1161     | 4       | 0            |
| 1   | U     | 1108  | 0        | 1126     | 8       | 0            |
| 1   | UA    | 1108  | 0        | 1126     | 3       | 0            |
| 1   | UB    | 1108  | 0        | 1126     | 6       | 0            |
| 1   | UC    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | V     | 1108  | 0        | 1126     | 4       | 0            |
| 1   | VA    | 1143  | 0        | 1161     | 5       | 0            |
| 1   | VB    | 1104  | 0        | 1123     | 7       | 0            |
| 1   | VC    | 1127  | 0        | 1145     | 5       | 0            |
| 1   | W     | 1108  | 0        | 1126     | 6       | 0            |
| 1   | WA    | 1108  | 0        | 1126     | 2       | 0            |
| 1   | WB    | 1134  | 0        | 1153     | 6       | 0            |
| 1   | WC    | 1108  | 0        | 1126     | 8       | 0            |
| 1   | X     | 1104  | 0        | 1123     | 6       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | XA    | 1127   | 0        | 1146     | 4       | 0            |
| 1   | XB    | 1104   | 0        | 1123     | 7       | 0            |
| 1   | XC    | 1108   | 0        | 1126     | 4       | 0            |
| 1   | Y     | 1134   | 0        | 1153     | 6       | 0            |
| 1   | YA    | 1108   | 0        | 1126     | 8       | 0            |
| 1   | YB    | 1108   | 0        | 1126     | 2       | 0            |
| 1   | YC    | 1108   | 0        | 1126     | 6       | 0            |
| 1   | Z     | 1104   | 0        | 1123     | 7       | 0            |
| 1   | ZA    | 1108   | 0        | 1126     | 4       | 0            |
| 1   | ZB    | 1143   | 0        | 1161     | 5       | 0            |
| 1   | ZC    | 1104   | 0        | 1123     | 5       | 0            |
| All | All   | 133824 | 0        | 136031   | 458     | 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 2.

All (458) 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:A:27:GLU:OE1  | 1:L:84:ARG:NH1   | 2.14                     | 0.79              |
| 1:ZA:84:ARG:NH1 | 1:CC:27:GLU:OE1  | 2.16                     | 0.78              |
| 1:B:84:ARG:NH1  | 1:GD:27:GLU:OE1  | 2.16                     | 0.78              |
| 1:K:27:GLU:OE1  | 1:HD:84:ARG:NH1  | 2.17                     | 0.78              |
| 1:TB:84:ARG:NH1 | 1:MC:27:GLU:OE1  | 2.16                     | 0.78              |
| 1:U:27:GLU:OE1  | 1:DC:84:ARG:NH1  | 2.19                     | 0.75              |
| 1:FA:84:ARG:NH1 | 1:IB:27:GLU:OE1  | 2.18                     | 0.75              |
| 1:OA:27:GLU:OE1 | 1:JB:84:ARG:NH1  | 2.18                     | 0.75              |
| 1:EA:27:GLU:OE1 | 1:PA:84:ARG:NH1  | 2.19                     | 0.74              |
| 1:V:84:ARG:NH1  | 1:YA:27:GLU:OE1  | 2.20                     | 0.74              |
| 1:NC:84:ARG:NH1 | 1:WC:27:GLU:OE1  | 2.20                     | 0.73              |
| 1:SB:27:GLU:OE1 | 1:XC:84:ARG:NH1  | 2.21                     | 0.73              |
| 1:Y:12:THR:HB   | 1:BA:23:LEU:HD11 | 1.74                     | 0.69              |
| 1:SA:12:THR:HB  | 1:VA:23:LEU:HD11 | 1.74                     | 0.69              |
| 1:GC:12:THR:HB  | 1:JC:23:LEU:HD11 | 1.74                     | 0.69              |
| 1:O:12:THR:HB   | 1:R:23:LEU:HD11  | 1.74                     | 0.69              |
| 1:MB:12:THR:HB  | 1:PB:23:LEU:HD11 | 1.74                     | 0.69              |
| 1:QC:12:THR:HB  | 1:TC:23:LEU:HD11 | 1.74                     | 0.69              |
| 1:E:12:THR:HB   | 1:H:23:LEU:HD11  | 1.74                     | 0.68              |
| 1:CB:12:THR:HB  | 1:FB:23:LEU:HD11 | 1.74                     | 0.68              |
| 1:IA:12:THR:HB  | 1:LA:23:LEU:HD11 | 1.74                     | 0.68              |
| 1:KD:12:THR:HB  | 1:ND:23:LEU:HD11 | 1.74                     | 0.68              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:AD:12:THR:HB  | 1:DD:23:LEU:HD11 | 1.74                     | 0.68              |
| 1:WB:12:THR:HB  | 1:ZB:23:LEU:HD11 | 1.74                     | 0.68              |
| 1:SA:138:SER:OG | 1:SA:142:LYS:NZ  | 2.29                     | 0.66              |
| 1:O:138:SER:OG  | 1:O:142:LYS:NZ   | 2.29                     | 0.66              |
| 1:IA:138:SER:OG | 1:IA:142:LYS:NZ  | 2.29                     | 0.66              |
| 1:KD:138:SER:OG | 1:KD:142:LYS:NZ  | 2.29                     | 0.66              |
| 1:MB:138:SER:OG | 1:MB:142:LYS:NZ  | 2.29                     | 0.66              |
| 1:WB:138:SER:OG | 1:WB:142:LYS:NZ  | 2.29                     | 0.66              |
| 1:AD:138:SER:OG | 1:AD:142:LYS:NZ  | 2.29                     | 0.65              |
| 1:K:84:ARG:NH1  | 1:HD:27:GLU:OE2  | 2.29                     | 0.65              |
| 1:Y:138:SER:OG  | 1:Y:142:LYS:NZ   | 2.29                     | 0.65              |
| 1:CB:138:SER:OG | 1:CB:142:LYS:NZ  | 2.29                     | 0.65              |
| 1:GC:138:SER:OG | 1:GC:142:LYS:NZ  | 2.29                     | 0.65              |
| 1:E:138:SER:OG  | 1:E:142:LYS:NZ   | 2.29                     | 0.65              |
| 1:QC:138:SER:OG | 1:QC:142:LYS:NZ  | 2.29                     | 0.65              |
| 1:U:84:ARG:NH1  | 1:DC:27:GLU:OE2  | 2.29                     | 0.65              |
| 1:OA:84:ARG:NH1 | 1:JB:27:GLU:OE2  | 2.31                     | 0.64              |
| 1:NB:138:SER:OG | 1:NB:142:LYS:NZ  | 2.32                     | 0.63              |
| 1:HC:138:SER:OG | 1:HC:142:LYS:NZ  | 2.32                     | 0.63              |
| 1:P:138:SER:OG  | 1:P:142:LYS:NZ   | 2.32                     | 0.63              |
| 1:XB:138:SER:OG | 1:XB:142:LYS:NZ  | 2.32                     | 0.63              |
| 1:RC:138:SER:OG | 1:RC:142:LYS:NZ  | 2.32                     | 0.63              |
| 1:LD:138:SER:OG | 1:LD:142:LYS:NZ  | 2.32                     | 0.63              |
| 1:F:138:SER:OG  | 1:F:142:LYS:NZ   | 2.32                     | 0.63              |
| 1:V:27:GLU:OE2  | 1:YA:84:ARG:NH1  | 2.32                     | 0.62              |
| 1:TA:138:SER:OG | 1:TA:142:LYS:NZ  | 2.32                     | 0.62              |
| 1:Z:138:SER:OG  | 1:Z:142:LYS:NZ   | 2.32                     | 0.62              |
| 1:JA:138:SER:OG | 1:JA:142:LYS:NZ  | 2.32                     | 0.62              |
| 1:BD:138:SER:OG | 1:BD:142:LYS:NZ  | 2.32                     | 0.62              |
| 1:DB:138:SER:OG | 1:DB:142:LYS:NZ  | 2.32                     | 0.62              |
| 1:EA:84:ARG:NH1 | 1:PA:27:GLU:OE2  | 2.33                     | 0.61              |
| 1:A:84:ARG:NH1  | 1:L:27:GLU:OE2   | 2.34                     | 0.61              |
| 1:ZA:27:GLU:OE2 | 1:CC:84:ARG:NH1  | 2.34                     | 0.61              |
| 1:TB:27:GLU:OE2 | 1:MC:84:ARG:NH1  | 2.35                     | 0.60              |
| 1:NC:27:GLU:OE2 | 1:WC:84:ARG:NH1  | 2.33                     | 0.60              |
| 1:FA:27:GLU:OE2 | 1:IB:84:ARG:NH1  | 2.35                     | 0.60              |
| 1:ED:49:GLU:OE2 | 1:FD:65:ARG:NH2  | 2.36                     | 0.59              |
| 1:B:27:GLU:OE2  | 1:GD:84:ARG:NH1  | 2.35                     | 0.59              |
| 1:S:49:GLU:OE2  | 1:T:65:ARG:NH2   | 2.36                     | 0.58              |
| 1:QC:12:THR:HG1 | 1:QC:19:TRP:HE1  | 1.50                     | 0.58              |
| 1:QB:49:GLU:OE2 | 1:RB:65:ARG:NH2  | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UC:49:GLU:OE2   | 1:VC:65:ARG:NH2   | 2.36                     | 0.58              |
| 1:U:84:ARG:NH1    | 1:EC:65:ARG:HH12  | 2.01                     | 0.58              |
| 1:WA:49:GLU:OE2   | 1:XA:65:ARG:NH2   | 2.36                     | 0.57              |
| 1:CA:49:GLU:OE2   | 1:DA:65:ARG:NH2   | 2.36                     | 0.57              |
| 1:SB:84:ARG:NH1   | 1:XC:27:GLU:OE2   | 2.37                     | 0.57              |
| 1:KC:49:GLU:OE2   | 1:LC:65:ARG:NH2   | 2.36                     | 0.57              |
| 1:Y:12:THR:HG1    | 1:Y:19:TRP:HE1    | 1.53                     | 0.57              |
| 1:MA:49:GLU:OE2   | 1:NA:65:ARG:NH2   | 2.36                     | 0.56              |
| 1:I:49:GLU:OE2    | 1:J:65:ARG:NH2    | 2.36                     | 0.56              |
| 1:GB:49:GLU:OE2   | 1:HB:65:ARG:NH2   | 2.36                     | 0.56              |
| 1:OD:49:GLU:OE2   | 1:PD:65:ARG:NH2   | 2.36                     | 0.56              |
| 1:MB:12:THR:HG1   | 1:MB:19:TRP:HE1   | 1.54                     | 0.56              |
| 1:E:12:THR:HG1    | 1:E:19:TRP:HE1    | 1.54                     | 0.55              |
| 1:U:84:ARG:NH1    | 1:EC:65:ARG:NH1   | 2.54                     | 0.55              |
| 1:W:65:ARG:HH12   | 1:YA:84:ARG:NH1   | 2.05                     | 0.54              |
| 1:C:67:ASN:OD1    | 1:C:68:HIS:N      | 2.41                     | 0.54              |
| 1:OC:67:ASN:OD1   | 1:OC:68:HIS:N     | 2.41                     | 0.54              |
| 1:GA:67:ASN:OD1   | 1:GA:68:HIS:N     | 2.41                     | 0.54              |
| 1:YA:108:GLY:CA   | 1:YA:147:LEU:HD21 | 2.38                     | 0.54              |
| 1:AB:67:ASN:OD1   | 1:AB:68:HIS:N     | 2.41                     | 0.54              |
| 1:RB:125:LEU:HD13 | 1:RB:159:VAL:CG1  | 2.38                     | 0.54              |
| 1:EC:67:ASN:OD1   | 1:EC:68:HIS:N     | 2.41                     | 0.54              |
| 1:U:108:GLY:CA    | 1:U:147:LEU:HD21  | 2.38                     | 0.54              |
| 1:AC:49:GLU:OE2   | 1:BC:65:ARG:NH2   | 2.36                     | 0.54              |
| 1:J:125:LEU:HD13  | 1:J:159:VAL:CG1   | 2.38                     | 0.54              |
| 1:OA:84:ARG:NH1   | 1:KB:65:ARG:HH12  | 2.05                     | 0.54              |
| 1:FD:125:LEU:HD13 | 1:FD:159:VAL:CG1  | 2.38                     | 0.54              |
| 1:KB:67:ASN:OD1   | 1:KB:68:HIS:N     | 2.41                     | 0.54              |
| 1:BC:125:LEU:HD13 | 1:BC:159:VAL:CG1  | 2.38                     | 0.54              |
| 1:A:108:GLY:CA    | 1:A:147:LEU:HD21  | 2.38                     | 0.54              |
| 1:C:50:GLY:O      | 1:MD:84:ARG:NH2   | 2.39                     | 0.54              |
| 1:W:67:ASN:OD1    | 1:W:68:HIS:N      | 2.41                     | 0.54              |
| 1:OA:108:GLY:CA   | 1:OA:147:LEU:HD21 | 2.38                     | 0.54              |
| 1:CC:108:GLY:CA   | 1:CC:147:LEU:HD21 | 2.38                     | 0.54              |
| 1:LC:125:LEU:HD13 | 1:LC:159:VAL:CG1  | 2.38                     | 0.54              |
| 1:YC:67:ASN:OD1   | 1:YC:68:HIS:N     | 2.41                     | 0.54              |
| 1:GD:108:GLY:CA   | 1:GD:147:LEU:HD21 | 2.38                     | 0.54              |
| 1:PD:125:LEU:HD13 | 1:PD:159:VAL:CG1  | 2.38                     | 0.54              |
| 1:T:125:LEU:HD13  | 1:T:159:VAL:CG1   | 2.38                     | 0.54              |
| 1:EA:108:GLY:CA   | 1:EA:147:LEU:HD21 | 2.38                     | 0.54              |
| 1:W:65:ARG:NH1    | 1:YA:84:ARG:NH1   | 2.56                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:12:THR:HG1    | 1:O:19:TRP:HE1    | 1.57                     | 0.53              |
| 1:XA:125:LEU:HD13 | 1:XA:159:VAL:CG1  | 2.38                     | 0.53              |
| 1:M:67:ASN:OD1    | 1:M:68:HIS:N      | 2.41                     | 0.53              |
| 1:NA:125:LEU:HD13 | 1:NA:159:VAL:CG1  | 2.38                     | 0.53              |
| 1:LA:12:THR:HG22  | 1:LA:77:GLY:HA2   | 1.91                     | 0.53              |
| 1:AB:65:ARG:HH12  | 1:CC:84:ARG:NH1   | 2.07                     | 0.53              |
| 1:CB:12:THR:HG1   | 1:CB:19:TRP:HE1   | 1.55                     | 0.53              |
| 1:K:108:GLY:CA    | 1:K:147:LEU:HD21  | 2.38                     | 0.53              |
| 1:DA:125:LEU:HD13 | 1:DA:159:VAL:CG1  | 2.38                     | 0.53              |
| 1:HB:125:LEU:HD13 | 1:HB:159:VAL:CG1  | 2.38                     | 0.53              |
| 1:UB:67:ASN:OD1   | 1:UB:68:HIS:N     | 2.41                     | 0.53              |
| 1:VC:125:LEU:HD13 | 1:VC:159:VAL:CG1  | 2.38                     | 0.53              |
| 1:WC:108:GLY:CA   | 1:WC:147:LEU:HD21 | 2.38                     | 0.53              |
| 1:BA:12:THR:HG22  | 1:BA:77:GLY:HA2   | 1.91                     | 0.53              |
| 1:QA:67:ASN:OD1   | 1:QA:68:HIS:N     | 2.41                     | 0.53              |
| 1:VA:12:THR:HG22  | 1:VA:77:GLY:HA2   | 1.91                     | 0.53              |
| 1:PB:12:THR:HG22  | 1:PB:77:GLY:HA2   | 1.91                     | 0.53              |
| 1:SB:108:GLY:CA   | 1:SB:147:LEU:HD21 | 2.38                     | 0.53              |
| 1:OC:65:ARG:HH12  | 1:WC:84:ARG:NH1   | 2.06                     | 0.53              |
| 1:ID:67:ASN:OD1   | 1:ID:68:HIS:N     | 2.41                     | 0.53              |
| 1:EA:84:ARG:NH1   | 1:QA:65:ARG:HH12  | 2.07                     | 0.53              |
| 1:BD:22:ALA:O     | 1:BD:26:ILE:HD12  | 2.09                     | 0.53              |
| 1:ZB:12:THR:HG22  | 1:ZB:77:GLY:HA2   | 1.91                     | 0.53              |
| 1:MC:108:GLY:CA   | 1:MC:147:LEU:HD21 | 2.38                     | 0.53              |
| 1:LD:22:ALA:O     | 1:LD:26:ILE:HD12  | 2.09                     | 0.53              |
| 1:TA:22:ALA:O     | 1:TA:26:ILE:HD12  | 2.09                     | 0.52              |
| 1:R:12:THR:HG22   | 1:R:77:GLY:HA2    | 1.91                     | 0.52              |
| 1:XB:22:ALA:O     | 1:XB:26:ILE:HD12  | 2.10                     | 0.52              |
| 1:OC:65:ARG:NH1   | 1:WC:84:ARG:NH1   | 2.58                     | 0.52              |
| 1:P:132:HIS:NE2   | 1:T:159:VAL:O     | 2.43                     | 0.52              |
| 1:Z:132:HIS:NE2   | 1:DA:159:VAL:O    | 2.43                     | 0.52              |
| 1:DD:12:THR:HG22  | 1:DD:77:GLY:HA2   | 1.91                     | 0.52              |
| 1:ND:12:THR:HG22  | 1:ND:77:GLY:HA2   | 1.91                     | 0.52              |
| 1:XB:132:HIS:NE2  | 1:BC:159:VAL:O    | 2.43                     | 0.52              |
| 1:TC:12:THR:HG22  | 1:TC:77:GLY:HA2   | 1.91                     | 0.52              |
| 1:TA:132:HIS:NE2  | 1:XA:159:VAL:O    | 2.43                     | 0.52              |
| 1:IB:108:GLY:CA   | 1:IB:147:LEU:HD21 | 2.38                     | 0.52              |
| 1:NB:22:ALA:O     | 1:NB:26:ILE:HD12  | 2.09                     | 0.52              |
| 1:NB:132:HIS:NE2  | 1:RB:159:VAL:O    | 2.43                     | 0.52              |
| 1:GC:12:THR:HG1   | 1:GC:19:TRP:HE1   | 1.58                     | 0.52              |
| 1:RC:132:HIS:NE2  | 1:VC:159:VAL:O    | 2.43                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:132:HIS:NE2   | 1:J:159:VAL:O     | 2.43                     | 0.52              |
| 1:Z:22:ALA:O      | 1:Z:26:ILE:HD12   | 2.10                     | 0.52              |
| 1:JA:132:HIS:NE2  | 1:NA:159:VAL:O    | 2.43                     | 0.52              |
| 1:FB:12:THR:HG22  | 1:FB:77:GLY:HA2   | 1.91                     | 0.52              |
| 1:RC:22:ALA:O     | 1:RC:26:ILE:HD12  | 2.09                     | 0.52              |
| 1:BD:132:HIS:NE2  | 1:FD:159:VAL:O    | 2.43                     | 0.52              |
| 1:SA:12:THR:HG1   | 1:SA:19:TRP:HE1   | 1.58                     | 0.52              |
| 1:DC:27:GLU:OE2   | 1:EC:65:ARG:NH1   | 2.43                     | 0.52              |
| 1:H:12:THR:HG22   | 1:H:77:GLY:HA2    | 1.91                     | 0.51              |
| 1:JC:12:THR:HG22  | 1:JC:77:GLY:HA2   | 1.91                     | 0.51              |
| 1:F:22:ALA:O      | 1:F:26:ILE:HD12   | 2.09                     | 0.51              |
| 1:K:84:ARG:NH1    | 1:ID:65:ARG:HH12  | 2.07                     | 0.51              |
| 1:FA:27:GLU:OE2   | 1:GA:65:ARG:NH1   | 2.43                     | 0.51              |
| 1:JA:22:ALA:O     | 1:JA:26:ILE:HD12  | 2.10                     | 0.51              |
| 1:DB:22:ALA:O     | 1:DB:26:ILE:HD12  | 2.10                     | 0.51              |
| 1:HC:22:ALA:O     | 1:HC:26:ILE:HD12  | 2.09                     | 0.51              |
| 1:L:27:GLU:OE2    | 1:M:65:ARG:NH1    | 2.43                     | 0.51              |
| 1:GA:65:ARG:HH12  | 1:IB:84:ARG:NH1   | 2.09                     | 0.51              |
| 1:P:22:ALA:O      | 1:P:26:ILE:HD12   | 2.09                     | 0.51              |
| 1:ZA:27:GLU:OE2   | 1:AB:65:ARG:NH1   | 2.43                     | 0.51              |
| 1:V:27:GLU:OE2    | 1:W:65:ARG:NH1    | 2.43                     | 0.51              |
| 1:LD:132:HIS:NE2  | 1:PD:159:VAL:O    | 2.43                     | 0.51              |
| 1:DB:132:HIS:NE2  | 1:HB:159:VAL:O    | 2.43                     | 0.51              |
| 1:HC:132:HIS:NE2  | 1:LC:159:VAL:O    | 2.43                     | 0.51              |
| 1:XC:27:GLU:OE2   | 1:YC:65:ARG:NH1   | 2.43                     | 0.51              |
| 1:B:27:GLU:OE2    | 1:C:65:ARG:NH1    | 2.43                     | 0.51              |
| 1:PA:27:GLU:OE2   | 1:QA:65:ARG:NH1   | 2.43                     | 0.51              |
| 1:JB:27:GLU:OE2   | 1:KB:65:ARG:NH1   | 2.43                     | 0.51              |
| 1:NC:27:GLU:OE2   | 1:OC:65:ARG:NH1   | 2.44                     | 0.51              |
| 1:Y:125:LEU:HD13  | 1:Y:159:VAL:HG13  | 1.94                     | 0.50              |
| 1:O:125:LEU:HD13  | 1:O:159:VAL:HG13  | 1.94                     | 0.50              |
| 1:IA:125:LEU:HD13 | 1:IA:159:VAL:HG13 | 1.94                     | 0.50              |
| 1:E:125:LEU:HD13  | 1:E:159:VAL:HG13  | 1.94                     | 0.50              |
| 1:K:84:ARG:NH1    | 1:ID:65:ARG:NH1   | 2.59                     | 0.50              |
| 1:TB:27:GLU:OE2   | 1:UB:65:ARG:NH1   | 2.43                     | 0.50              |
| 1:AD:125:LEU:HD13 | 1:AD:159:VAL:HG13 | 1.94                     | 0.50              |
| 1:EA:84:ARG:NH1   | 1:QA:65:ARG:NH1   | 2.59                     | 0.50              |
| 1:AB:65:ARG:NH1   | 1:CC:84:ARG:NH1   | 2.59                     | 0.50              |
| 1:QC:125:LEU:HD13 | 1:QC:159:VAL:HG13 | 1.94                     | 0.50              |
| 1:CB:125:LEU:HD13 | 1:CB:159:VAL:HG13 | 1.94                     | 0.50              |
| 1:GC:125:LEU:HD13 | 1:GC:159:VAL:HG13 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:KD:12:THR:HG1   | 1:KD:19:TRP:HE1   | 1.59                     | 0.50              |
| 1:KD:125:LEU:HD13 | 1:KD:159:VAL:HG13 | 1.94                     | 0.50              |
| 1:IA:12:THR:HG1   | 1:IA:19:TRP:HE1   | 1.58                     | 0.50              |
| 1:UA:84:ARG:NH2   | 1:KB:50:GLY:O     | 2.41                     | 0.50              |
| 1:UB:65:ARG:HH12  | 1:MC:84:ARG:NH1   | 2.10                     | 0.50              |
| 1:HD:27:GLU:OE2   | 1:ID:65:ARG:NH1   | 2.43                     | 0.50              |
| 1:OA:84:ARG:NH1   | 1:KB:65:ARG:NH1   | 2.59                     | 0.50              |
| 1:SA:125:LEU:HD13 | 1:SA:159:VAL:HG13 | 1.94                     | 0.50              |
| 1:MB:125:LEU:HD13 | 1:MB:159:VAL:HG13 | 1.94                     | 0.49              |
| 1:WB:125:LEU:HD13 | 1:WB:159:VAL:HG13 | 1.94                     | 0.49              |
| 1:U:85:HIS:CE1    | 1:DC:52:LEU:HD12  | 2.47                     | 0.49              |
| 1:UB:65:ARG:NH1   | 1:MC:84:ARG:NH1   | 2.61                     | 0.49              |
| 1:C:65:ARG:HH12   | 1:GD:84:ARG:NH1   | 2.11                     | 0.48              |
| 1:SB:84:ARG:NH1   | 1:YC:65:ARG:NH1   | 2.62                     | 0.48              |
| 1:GA:65:ARG:NH1   | 1:IB:84:ARG:NH1   | 2.62                     | 0.48              |
| 1:P:70:LEU:O      | 1:P:74:LEU:HD23   | 2.14                     | 0.48              |
| 1:Z:70:LEU:O      | 1:Z:74:LEU:HD23   | 2.14                     | 0.48              |
| 1:JA:70:LEU:O     | 1:JA:74:LEU:HD23  | 2.14                     | 0.48              |
| 1:A:84:ARG:NH1    | 1:M:65:ARG:HH12   | 2.11                     | 0.48              |
| 1:VB:16:ASN:O     | 1:VB:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:A:84:ARG:NH1    | 1:M:65:ARG:NH1    | 2.62                     | 0.47              |
| 1:D:16:ASN:O      | 1:D:19:TRP:NE1    | 2.47                     | 0.47              |
| 1:GA:50:GLY:O     | 1:OB:84:ARG:NH2   | 2.44                     | 0.47              |
| 1:LB:16:ASN:O     | 1:LB:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:NB:70:LEU:O     | 1:NB:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:TA:70:LEU:O     | 1:TA:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:AD:12:THR:HG1   | 1:AD:19:TRP:HE1   | 1.61                     | 0.47              |
| 1:BD:70:LEU:O     | 1:BD:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:BB:16:ASN:O     | 1:BB:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:DB:70:LEU:O     | 1:DB:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:SB:84:ARG:NH1   | 1:YC:65:ARG:HH12  | 2.11                     | 0.47              |
| 1:HC:70:LEU:O     | 1:HC:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:YC:44:SER:N     | 1:ZC:90:GLU:OE1   | 2.48                     | 0.47              |
| 1:ZC:16:ASN:O     | 1:ZC:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:X:16:ASN:O      | 1:X:19:TRP:NE1    | 2.47                     | 0.47              |
| 1:XB:70:LEU:O     | 1:XB:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:EC:44:SER:N     | 1:FC:90:GLU:OE1   | 2.48                     | 0.47              |
| 1:FC:16:ASN:O     | 1:FC:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:C:44:SER:N      | 1:D:90:GLU:OE1    | 2.48                     | 0.47              |
| 1:N:16:ASN:O      | 1:N:19:TRP:NE1    | 2.47                     | 0.47              |
| 1:W:44:SER:N      | 1:X:90:GLU:OE1    | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HA:16:ASN:O     | 1:HA:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:QA:44:SER:N     | 1:RA:90:GLU:OE1   | 2.48                     | 0.47              |
| 1:RA:16:ASN:O     | 1:RA:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:AB:44:SER:N     | 1:BB:90:GLU:OE1   | 2.48                     | 0.47              |
| 1:UB:44:SER:N     | 1:VB:90:GLU:OE1   | 2.48                     | 0.47              |
| 1:OC:44:SER:N     | 1:PC:90:GLU:OE1   | 2.48                     | 0.47              |
| 1:PC:16:ASN:O     | 1:PC:19:TRP:NE1   | 2.47                     | 0.47              |
| 1:F:70:LEU:O      | 1:F:74:LEU:HD23   | 2.14                     | 0.47              |
| 1:M:44:SER:N      | 1:N:90:GLU:OE1    | 2.48                     | 0.47              |
| 1:LD:70:LEU:O     | 1:LD:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:KB:44:SER:N     | 1:LB:90:GLU:OE1   | 2.48                     | 0.47              |
| 1:RC:70:LEU:O     | 1:RC:74:LEU:HD23  | 2.14                     | 0.47              |
| 1:CC:147:LEU:HD13 | 1:GC:149:LEU:HD12 | 1.98                     | 0.46              |
| 1:GA:44:SER:N     | 1:HA:90:GLU:OE1   | 2.48                     | 0.46              |
| 1:ID:44:SER:N     | 1:JD:90:GLU:OE1   | 2.48                     | 0.46              |
| 1:W:17:LYS:HD3    | 1:W:160:ILE:HG22  | 1.98                     | 0.46              |
| 1:YA:147:LEU:HD13 | 1:CB:149:LEU:HD12 | 1.98                     | 0.46              |
| 1:IB:147:LEU:HD13 | 1:MB:149:LEU:HD12 | 1.98                     | 0.46              |
| 1:SB:108:GLY:HA2  | 1:SB:147:LEU:HD21 | 1.98                     | 0.46              |
| 1:EC:17:LYS:HD3   | 1:EC:160:ILE:HG22 | 1.98                     | 0.46              |
| 1:JD:16:ASN:O     | 1:JD:19:TRP:NE1   | 2.47                     | 0.46              |
| 1:A:147:LEU:HD13  | 1:E:149:LEU:HD12  | 1.98                     | 0.46              |
| 1:EA:147:LEU:HD13 | 1:IA:149:LEU:HD12 | 1.98                     | 0.46              |
| 1:WC:147:LEU:HD13 | 1:AD:149:LEU:HD12 | 1.98                     | 0.46              |
| 1:YC:17:LYS:HD3   | 1:YC:160:ILE:HG22 | 1.98                     | 0.46              |
| 1:QA:17:LYS:HD3   | 1:QA:160:ILE:HG22 | 1.98                     | 0.46              |
| 1:RB:30:ASN:ND2   | 1:RB:51:LYS:O     | 2.49                     | 0.46              |
| 1:C:17:LYS:HD3    | 1:C:160:ILE:HG22  | 1.98                     | 0.46              |
| 1:J:30:ASN:ND2    | 1:J:51:LYS:O      | 2.49                     | 0.46              |
| 1:U:108:GLY:HA2   | 1:U:147:LEU:HD21  | 1.98                     | 0.46              |
| 1:DA:30:ASN:ND2   | 1:DA:51:LYS:O     | 2.49                     | 0.46              |
| 1:NA:30:ASN:ND2   | 1:NA:51:LYS:O     | 2.49                     | 0.46              |
| 1:SB:147:LEU:HD13 | 1:WB:149:LEU:HD12 | 1.98                     | 0.46              |
| 1:VC:30:ASN:ND2   | 1:VC:51:LYS:O     | 2.49                     | 0.46              |
| 1:CC:108:GLY:HA2  | 1:CC:147:LEU:HD21 | 1.98                     | 0.46              |
| 1:GD:147:LEU:HD13 | 1:KD:149:LEU:HD12 | 1.98                     | 0.46              |
| 1:M:17:LYS:HD3    | 1:M:160:ILE:HG22  | 1.98                     | 0.46              |
| 1:OA:85:HIS:CE1   | 1:JB:52:LEU:HD12  | 2.50                     | 0.46              |
| 1:GD:108:GLY:HA2  | 1:GD:147:LEU:HD21 | 1.98                     | 0.46              |
| 1:T:30:ASN:ND2    | 1:T:51:LYS:O      | 2.49                     | 0.45              |
| 1:U:147:LEU:HD13  | 1:Y:149:LEU:HD12  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HB:30:ASN:ND2   | 1:HB:51:LYS:O     | 2.49                     | 0.45              |
| 1:FD:30:ASN:ND2   | 1:FD:51:LYS:O     | 2.49                     | 0.45              |
| 1:VA:125:LEU:HD23 | 1:VA:159:VAL:CG1  | 2.47                     | 0.45              |
| 1:AB:17:LYS:HD3   | 1:AB:160:ILE:HG22 | 1.98                     | 0.45              |
| 1:UB:17:LYS:HD3   | 1:UB:160:ILE:HG22 | 1.98                     | 0.45              |
| 1:MC:108:GLY:HA2  | 1:MC:147:LEU:HD21 | 1.98                     | 0.45              |
| 1:DD:125:LEU:HD23 | 1:DD:159:VAL:CG1  | 2.47                     | 0.45              |
| 1:K:85:HIS:CE1    | 1:HD:52:LEU:HD12  | 2.51                     | 0.45              |
| 1:YA:108:GLY:HA2  | 1:YA:147:LEU:HD21 | 1.98                     | 0.45              |
| 1:LC:30:ASN:ND2   | 1:LC:51:LYS:O     | 2.49                     | 0.45              |
| 1:K:147:LEU:HD13  | 1:O:149:LEU:HD12  | 1.98                     | 0.45              |
| 1:R:125:LEU:HD23  | 1:R:159:VAL:CG1   | 2.47                     | 0.45              |
| 1:EA:108:GLY:HA2  | 1:EA:147:LEU:HD21 | 1.98                     | 0.45              |
| 1:GA:17:LYS:HD3   | 1:GA:160:ILE:HG22 | 1.98                     | 0.45              |
| 1:FC:125:LEU:HD13 | 1:FC:159:VAL:HG11 | 1.99                     | 0.45              |
| 1:ZB:125:LEU:HD23 | 1:ZB:159:VAL:CG1  | 2.47                     | 0.45              |
| 1:H:125:LEU:HD23  | 1:H:159:VAL:CG1   | 2.47                     | 0.45              |
| 1:OA:147:LEU:HD13 | 1:SA:149:LEU:HD12 | 1.98                     | 0.45              |
| 1:BB:125:LEU:HD13 | 1:BB:159:VAL:HG11 | 1.99                     | 0.45              |
| 1:KB:17:LYS:HD3   | 1:KB:160:ILE:HG22 | 1.98                     | 0.45              |
| 1:LB:125:LEU:HD13 | 1:LB:159:VAL:HG11 | 1.99                     | 0.45              |
| 1:ID:17:LYS:HD3   | 1:ID:160:ILE:HG22 | 1.98                     | 0.45              |
| 1:PD:30:ASN:ND2   | 1:PD:51:LYS:O     | 2.49                     | 0.45              |
| 1:A:108:GLY:HA2   | 1:A:147:LEU:HD21  | 1.98                     | 0.45              |
| 1:D:125:LEU:HD13  | 1:D:159:VAL:HG11  | 1.99                     | 0.45              |
| 1:BA:125:LEU:HD23 | 1:BA:159:VAL:CG1  | 2.47                     | 0.45              |
| 1:ZA:52:LEU:HD12  | 1:CC:85:HIS:CE1   | 2.52                     | 0.45              |
| 1:TC:125:LEU:HD23 | 1:TC:159:VAL:CG1  | 2.47                     | 0.45              |
| 1:K:108:GLY:HA2   | 1:K:147:LEU:HD21  | 1.98                     | 0.45              |
| 1:LA:125:LEU:HD23 | 1:LA:159:VAL:CG1  | 2.47                     | 0.45              |
| 1:XA:30:ASN:ND2   | 1:XA:51:LYS:O     | 2.49                     | 0.45              |
| 1:IB:108:GLY:HA2  | 1:IB:147:LEU:HD21 | 1.98                     | 0.45              |
| 1:JD:125:LEU:HD13 | 1:JD:159:VAL:HG11 | 1.99                     | 0.45              |
| 1:H:12:THR:HG22   | 1:H:77:GLY:CA     | 2.48                     | 0.44              |
| 1:OA:108:GLY:HA2  | 1:OA:147:LEU:HD21 | 1.98                     | 0.44              |
| 1:RA:125:LEU:HD13 | 1:RA:159:VAL:HG11 | 1.99                     | 0.44              |
| 1:JC:125:LEU:HD23 | 1:JC:159:VAL:CG1  | 2.47                     | 0.44              |
| 1:WC:108:GLY:HA2  | 1:WC:147:LEU:HD21 | 1.98                     | 0.44              |
| 1:ZC:125:LEU:HD13 | 1:ZC:159:VAL:HG11 | 1.99                     | 0.44              |
| 1:BA:12:THR:HG22  | 1:BA:77:GLY:CA    | 2.48                     | 0.44              |
| 1:WB:126:ILE:HG23 | 1:WB:126:ILE:O    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BC:30:ASN:ND2   | 1:BC:51:LYS:O     | 2.49                     | 0.44              |
| 1:OC:17:LYS:HD3   | 1:OC:160:ILE:HG22 | 1.98                     | 0.44              |
| 1:C:65:ARG:NH1    | 1:GD:84:ARG:NH1   | 2.65                     | 0.44              |
| 1:O:126:ILE:HG23  | 1:O:126:ILE:O     | 2.18                     | 0.44              |
| 1:FB:12:THR:HG22  | 1:FB:77:GLY:CA    | 2.48                     | 0.44              |
| 1:PC:125:LEU:HD13 | 1:PC:159:VAL:HG11 | 1.99                     | 0.44              |
| 1:TC:12:THR:HG22  | 1:TC:77:GLY:CA    | 2.48                     | 0.44              |
| 1:D:125:LEU:HD13  | 1:D:159:VAL:CG1   | 2.48                     | 0.44              |
| 1:N:125:LEU:HD13  | 1:N:159:VAL:CG1   | 2.48                     | 0.44              |
| 1:X:125:LEU:HD13  | 1:X:159:VAL:HG11  | 1.99                     | 0.44              |
| 1:UA:159:VAL:O    | 1:VA:132:HIS:ND1  | 2.49                     | 0.44              |
| 1:CB:126:ILE:O    | 1:CB:126:ILE:HG23 | 2.18                     | 0.44              |
| 1:XB:20:GLU:OE1   | 1:XB:20:GLU:N     | 2.37                     | 0.44              |
| 1:QC:126:ILE:O    | 1:QC:126:ILE:HG23 | 2.18                     | 0.44              |
| 1:CD:159:VAL:O    | 1:DD:132:HIS:ND1  | 2.49                     | 0.44              |
| 1:KD:126:ILE:HG23 | 1:KD:126:ILE:O    | 2.18                     | 0.44              |
| 1:V:52:LEU:HD12   | 1:YA:85:HIS:CE1   | 2.52                     | 0.44              |
| 1:EA:85:HIS:CE1   | 1:PA:52:LEU:HD12  | 2.52                     | 0.44              |
| 1:FB:125:LEU:HD23 | 1:FB:159:VAL:CG1  | 2.47                     | 0.44              |
| 1:OB:159:VAL:O    | 1:PB:132:HIS:ND1  | 2.49                     | 0.44              |
| 1:PB:125:LEU:HD23 | 1:PB:159:VAL:CG1  | 2.47                     | 0.44              |
| 1:MC:147:LEU:HD13 | 1:QC:149:LEU:HD12 | 1.98                     | 0.44              |
| 1:BD:49:GLU:OE2   | 1:CD:65:ARG:NH1   | 2.51                     | 0.44              |
| 1:ND:125:LEU:HD23 | 1:ND:159:VAL:CG1  | 2.47                     | 0.44              |
| 1:N:125:LEU:HD13  | 1:N:159:VAL:HG11  | 1.99                     | 0.44              |
| 1:IA:126:ILE:HG23 | 1:IA:126:ILE:O    | 2.18                     | 0.44              |
| 1:BB:125:LEU:HD13 | 1:BB:159:VAL:CG1  | 2.48                     | 0.44              |
| 1:VB:125:LEU:HD13 | 1:VB:159:VAL:CG1  | 2.48                     | 0.44              |
| 1:ZB:12:THR:HG22  | 1:ZB:77:GLY:CA    | 2.48                     | 0.44              |
| 1:X:125:LEU:HD13  | 1:X:159:VAL:CG1   | 2.48                     | 0.44              |
| 1:FA:52:LEU:HD12  | 1:IB:85:HIS:CE1   | 2.53                     | 0.44              |
| 1:HA:125:LEU:HD13 | 1:HA:159:VAL:HG11 | 1.99                     | 0.44              |
| 1:MB:126:ILE:O    | 1:MB:126:ILE:HG23 | 2.18                     | 0.44              |
| 1:VB:125:LEU:HD13 | 1:VB:159:VAL:HG11 | 1.99                     | 0.44              |
| 1:PC:125:LEU:HD13 | 1:PC:159:VAL:CG1  | 2.48                     | 0.44              |
| 1:DD:12:THR:HG22  | 1:DD:77:GLY:CA    | 2.48                     | 0.44              |
| 1:R:12:THR:HG22   | 1:R:77:GLY:CA     | 2.48                     | 0.44              |
| 1:LA:12:THR:HG22  | 1:LA:77:GLY:CA    | 2.48                     | 0.44              |
| 1:DB:49:GLU:OE2   | 1:EB:65:ARG:NH1   | 2.51                     | 0.44              |
| 1:IC:159:VAL:O    | 1:JC:132:HIS:ND1  | 2.49                     | 0.44              |
| 1:HA:125:LEU:HD13 | 1:HA:159:VAL:CG1  | 2.48                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:LB:125:LEU:HD13 | 1:LB:159:VAL:CG1 | 2.48                     | 0.43              |
| 1:WB:12:THR:HG1   | 1:WB:19:TRP:HE1  | 1.64                     | 0.43              |
| 1:Z:20:GLU:OE1    | 1:Z:20:GLU:N     | 2.37                     | 0.43              |
| 1:FC:125:LEU:HD13 | 1:FC:159:VAL:CG1 | 2.48                     | 0.43              |
| 1:RA:125:LEU:HD13 | 1:RA:159:VAL:CG1 | 2.48                     | 0.43              |
| 1:NC:52:LEU:HD12  | 1:WC:85:HIS:CE1  | 2.53                     | 0.43              |
| 1:MD:159:VAL:O    | 1:ND:132:HIS:ND1 | 2.49                     | 0.43              |
| 1:VA:12:THR:HG22  | 1:VA:77:GLY:CA   | 2.48                     | 0.43              |
| 1:HC:49:GLU:OE2   | 1:IC:65:ARG:NH1  | 2.51                     | 0.43              |
| 1:AD:126:ILE:HG23 | 1:AD:126:ILE:O   | 2.18                     | 0.43              |
| 1:PB:12:THR:HG22  | 1:PB:77:GLY:CA   | 2.48                     | 0.43              |
| 1:JC:12:THR:HG22  | 1:JC:77:GLY:CA   | 2.48                     | 0.43              |
| 1:ZC:125:LEU:HD13 | 1:ZC:159:VAL:CG1 | 2.48                     | 0.43              |
| 1:XB:49:GLU:OE2   | 1:YB:65:ARG:NH1  | 2.51                     | 0.43              |
| 1:JD:125:LEU:HD13 | 1:JD:159:VAL:CG1 | 2.48                     | 0.43              |
| 1:Q:84:ARG:NH2    | 1:ID:50:GLY:O    | 2.46                     | 0.43              |
| 1:Y:126:ILE:HG23  | 1:Y:126:ILE:O    | 2.18                     | 0.43              |
| 1:ND:12:THR:HG22  | 1:ND:77:GLY:CA   | 2.48                     | 0.43              |
| 1:B:52:LEU:HD12   | 1:GD:85:HIS:CE1  | 2.54                     | 0.43              |
| 1:GC:126:ILE:HG23 | 1:GC:126:ILE:O   | 2.18                     | 0.43              |
| 1:OD:130:THR:N    | 1:OD:131:PRO:HD2 | 2.34                     | 0.43              |
| 1:P:49:GLU:OE2    | 1:Q:65:ARG:NH1   | 2.51                     | 0.43              |
| 1:SA:126:ILE:HG23 | 1:SA:126:ILE:O   | 2.18                     | 0.43              |
| 1:E:126:ILE:HG23  | 1:E:126:ILE:O    | 2.18                     | 0.42              |
| 1:F:20:GLU:OE1    | 1:F:20:GLU:N     | 2.37                     | 0.42              |
| 1:S:130:THR:N     | 1:S:131:PRO:HD2  | 2.34                     | 0.42              |
| 1:DB:20:GLU:OE1   | 1:DB:20:GLU:N    | 2.37                     | 0.42              |
| 1:UC:130:THR:N    | 1:UC:131:PRO:HD2 | 2.34                     | 0.42              |
| 1:XB:78:ALA:O     | 1:XB:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:HC:78:ALA:O     | 1:HC:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:LD:49:GLU:OE2   | 1:MD:65:ARG:NH1  | 2.51                     | 0.42              |
| 1:P:78:ALA:O      | 1:P:82:ILE:HD12  | 2.20                     | 0.42              |
| 1:KA:84:ARG:NH2   | 1:QA:50:GLY:O    | 2.44                     | 0.42              |
| 1:MA:130:THR:N    | 1:MA:131:PRO:HD2 | 2.34                     | 0.42              |
| 1:JA:20:GLU:OE1   | 1:JA:20:GLU:N    | 2.37                     | 0.42              |
| 1:NB:78:ALA:O     | 1:NB:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:JA:78:ALA:O     | 1:JA:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:WA:130:THR:N    | 1:WA:131:PRO:HD2 | 2.34                     | 0.42              |
| 1:QB:130:THR:N    | 1:QB:131:PRO:HD2 | 2.34                     | 0.42              |
| 1:AC:130:THR:N    | 1:AC:131:PRO:HD2 | 2.34                     | 0.42              |
| 1:KC:130:THR:N    | 1:KC:131:PRO:HD2 | 2.34                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:ED:130:THR:N    | 1:ED:131:PRO:HD2 | 2.34                     | 0.42              |
| 1:F:49:GLU:OE2    | 1:G:65:ARG:NH1   | 2.51                     | 0.42              |
| 1:Z:49:GLU:OE2    | 1:AA:65:ARG:NH1  | 2.51                     | 0.42              |
| 1:BD:78:ALA:O     | 1:BD:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:Z:78:ALA:O      | 1:Z:82:ILE:HD12  | 2.20                     | 0.42              |
| 1:YB:159:VAL:O    | 1:ZB:132:HIS:ND1 | 2.49                     | 0.42              |
| 1:KA:159:VAL:O    | 1:LA:132:HIS:ND1 | 2.49                     | 0.42              |
| 1:TA:20:GLU:OE1   | 1:TA:20:GLU:N    | 2.37                     | 0.42              |
| 1:TA:49:GLU:OE2   | 1:UA:65:ARG:NH1  | 2.51                     | 0.42              |
| 1:DB:78:ALA:O     | 1:DB:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:NB:20:GLU:OE1   | 1:NB:20:GLU:N    | 2.37                     | 0.42              |
| 1:RC:78:ALA:O     | 1:RC:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:F:78:ALA:O      | 1:F:82:ILE:HD12  | 2.20                     | 0.42              |
| 1:TA:78:ALA:O     | 1:TA:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:LD:78:ALA:O     | 1:LD:82:ILE:HD12 | 2.20                     | 0.42              |
| 1:I:130:THR:N     | 1:I:131:PRO:HD2  | 2.34                     | 0.41              |
| 1:CA:130:THR:N    | 1:CA:131:PRO:HD2 | 2.34                     | 0.41              |
| 1:D:75:VAL:O      | 1:D:79:ILE:HD12  | 2.21                     | 0.41              |
| 1:BB:75:VAL:O     | 1:BB:79:ILE:HD12 | 2.21                     | 0.41              |
| 1:N:75:VAL:O      | 1:N:79:ILE:HD12  | 2.21                     | 0.41              |
| 1:RA:75:VAL:O     | 1:RA:79:ILE:HD12 | 2.20                     | 0.41              |
| 1:LC:13:LYS:O     | 1:LC:15:GLY:N    | 2.54                     | 0.41              |
| 1:JD:136:ILE:HD12 | 1:JD:136:ILE:H   | 1.86                     | 0.41              |
| 1:BB:136:ILE:HD12 | 1:BB:136:ILE:H   | 1.86                     | 0.41              |
| 1:FC:136:ILE:HD12 | 1:FC:136:ILE:H   | 1.86                     | 0.41              |
| 1:PC:75:VAL:O     | 1:PC:79:ILE:HD12 | 2.21                     | 0.41              |
| 1:PC:136:ILE:HD12 | 1:PC:136:ILE:H   | 1.86                     | 0.41              |
| 1:JA:49:GLU:OE2   | 1:KA:65:ARG:NH1  | 2.51                     | 0.41              |
| 1:FC:75:VAL:O     | 1:FC:79:ILE:HD12 | 2.21                     | 0.41              |
| 1:ZC:75:VAL:O     | 1:ZC:79:ILE:HD12 | 2.21                     | 0.41              |
| 1:FD:13:LYS:O     | 1:FD:15:GLY:N    | 2.54                     | 0.41              |
| 1:GB:130:THR:N    | 1:GB:131:PRO:HD2 | 2.34                     | 0.41              |
| 1:VC:13:LYS:O     | 1:VC:15[A]:GLY:N | 2.54                     | 0.41              |
| 1:LD:20:GLU:OE1   | 1:LD:20:GLU:N    | 2.37                     | 0.41              |
| 1:PD:13:LYS:O     | 1:PD:15:GLY:N    | 2.54                     | 0.41              |
| 1:X:75:VAL:O      | 1:X:79:ILE:HD12  | 2.21                     | 0.41              |
| 1:DA:13:LYS:O     | 1:DA:15:GLY:N    | 2.54                     | 0.41              |
| 1:RA:79:ILE:HD12  | 1:RA:79:ILE:H    | 1.86                     | 0.41              |
| 1:RA:136:ILE:HD12 | 1:RA:136:ILE:H   | 1.86                     | 0.41              |
| 1:LB:75:VAL:O     | 1:LB:79:ILE:HD12 | 2.20                     | 0.41              |
| 1:NB:49:GLU:OE2   | 1:OB:65:ARG:NH1  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:VB:136:ILE:HD12 | 1:VB:136:ILE:H    | 1.86                     | 0.41              |
| 1:RC:20:GLU:OE1   | 1:RC:20:GLU:N     | 2.37                     | 0.41              |
| 1:JD:79:ILE:HD12  | 1:JD:79:ILE:H     | 1.86                     | 0.41              |
| 1:Q:159:VAL:O     | 1:R:132:HIS:ND1   | 2.49                     | 0.41              |
| 1:HA:79:ILE:HD12  | 1:HA:79:ILE:H     | 1.86                     | 0.41              |
| 1:BC:13:LYS:O     | 1:BC:15:GLY:N     | 2.54                     | 0.41              |
| 1:JD:75:VAL:O     | 1:JD:79:ILE:HD12  | 2.21                     | 0.41              |
| 1:HA:75:VAL:O     | 1:HA:79:ILE:HD12  | 2.21                     | 0.40              |
| 1:BB:79:ILE:HD12  | 1:BB:79:ILE:H     | 1.86                     | 0.40              |
| 1:LB:79:ILE:HD12  | 1:LB:79:ILE:H     | 1.86                     | 0.40              |
| 1:VB:79:ILE:H     | 1:VB:79:ILE:HD12  | 1.86                     | 0.40              |
| 1:RC:49:GLU:OE2   | 1:SC:65:ARG:NH1   | 2.51                     | 0.40              |
| 1:AA:159:VAL:O    | 1:BA:132:HIS:ND1  | 2.49                     | 0.40              |
| 1:HA:136:ILE:HD12 | 1:HA:136:ILE:H    | 1.86                     | 0.40              |
| 1:TB:52:LEU:HD12  | 1:MC:85:HIS:CE1   | 2.56                     | 0.40              |
| 1:VB:75:VAL:O     | 1:VB:79:ILE:HD12  | 2.21                     | 0.40              |
| 1:N:79:ILE:HD12   | 1:N:79:ILE:H      | 1.86                     | 0.40              |
| 1:X:79:ILE:HD12   | 1:X:79:ILE:H      | 1.86                     | 0.40              |
| 1:LC:52:LEU:HD12  | 1:ED:85:HIS:CE1   | 2.56                     | 0.40              |
| 1:HB:13:LYS:O     | 1:HB:15:GLY:N     | 2.54                     | 0.40              |
| 1:RB:13:LYS:O     | 1:RB:15:GLY:N     | 2.54                     | 0.40              |
| 1:B:130:THR:O     | 1:B:132:HIS:N     | 2.55                     | 0.40              |
| 1:J:13:LYS:O      | 1:J:15:GLY:N      | 2.54                     | 0.40              |
| 1:DA:52:LEU:HD12  | 1:QB:85:HIS:CE1   | 2.57                     | 0.40              |
| 1:LB:136:ILE:H    | 1:LB:136:ILE:HD12 | 1.86                     | 0.40              |
| 1:XC:130:THR:O    | 1:XC:132:HIS:N    | 2.55                     | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | AA    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | AB    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | AC    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | AD    | 149/163 (91%) | 142 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 1   | B     | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | BA    | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | BB    | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | BC    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | BD    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | C     | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | CA    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | CB    | 149/163 (91%) | 143 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | CC    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | CD    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | D     | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | DA    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | DB    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | DC    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | DD    | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | E     | 149/163 (91%) | 142 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 1   | EA    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | EB    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | EC    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | ED    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | F     | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | FA    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | FB    | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | FC    | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | FD    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | G     | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | GA    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | GB    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | GC    | 149/163 (91%) | 142 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 1   | GD    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | H     | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | HA    | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | HB    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | HC    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | HD    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | I     | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | IA    | 149/163 (91%) | 142 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 1   | IB    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | IC    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | ID    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | J     | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | JA    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | JB    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | JC    | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | JD    | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | K     | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | KA    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | KB    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | KC    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | KD    | 149/163 (91%) | 143 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | L     | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | LA    | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | LB    | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | LC    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | LD    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | M     | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | MA    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | MB    | 149/163 (91%) | 142 (95%) | 7 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | MC    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | MD    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | N     | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | NA    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | NB    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | NC    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | ND    | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | O     | 149/163 (91%) | 143 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | OA    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | OB    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | OC    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | OD    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | P     | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | PA    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | PB    | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | PC    | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | PD    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | Q     | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | QA    | 146/163 (90%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | QB    | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | QC    | 149/163 (91%) | 143 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | R     | 151/163 (93%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | RA    | 145/163 (89%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | RB    | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | RC    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | S     | 146/163 (90%) | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | SA    | 149/163 (91%) | 143 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | SB    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | SC    | 146/163 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | T     | 148/163 (91%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | TA    | 145/163 (89%) | 140 (97%) | 5 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | TB    | 146/163 (90%)     | 137 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 1   | TC    | 151/163 (93%)     | 146 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 1   | U     | 146/163 (90%)     | 142 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 1   | UA    | 146/163 (90%)     | 142 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 1   | UB    | 146/163 (90%)     | 137 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 1   | UC    | 146/163 (90%)     | 143 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 1   | V     | 146/163 (90%)     | 137 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 1   | VA    | 151/163 (93%)     | 146 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 1   | VB    | 145/163 (89%)     | 142 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 1   | VC    | 148/163 (91%)     | 142 (96%)   | 6 (4%)   | 0        | 100         | 100 |
| 1   | W     | 146/163 (90%)     | 137 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 1   | WA    | 146/163 (90%)     | 143 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 1   | WB    | 149/163 (91%)     | 142 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 1   | WC    | 146/163 (90%)     | 142 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 1   | X     | 145/163 (89%)     | 142 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 1   | XA    | 148/163 (91%)     | 142 (96%)   | 6 (4%)   | 0        | 100         | 100 |
| 1   | XB    | 145/163 (89%)     | 140 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 1   | XC    | 146/163 (90%)     | 137 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 1   | Y     | 149/163 (91%)     | 142 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 1   | YA    | 146/163 (90%)     | 142 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 1   | YB    | 146/163 (90%)     | 142 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 1   | YC    | 146/163 (90%)     | 137 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 1   | Z     | 145/163 (89%)     | 140 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 1   | ZA    | 146/163 (90%)     | 137 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 1   | ZB    | 151/163 (93%)     | 146 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 1   | ZC    | 145/163 (89%)     | 142 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| All | All   | 17616/19560 (90%) | 16961 (96%) | 655 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AD    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | B     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BA    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | BB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BC    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | BD    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | C     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CB    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | CC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CD    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | D     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | DA    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | DB    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | DC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | DD    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | E     | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | EA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | EB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | EC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | ED    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | F     | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | FA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | FB    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | FC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | FD    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | G     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | GA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | GB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | GC    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | GD    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | H     | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | HA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | HB    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | HC    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | HD    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | I     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | IA    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | IB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | IC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | ID    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | J     | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | JA    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | JB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | JC    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | JD    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | K     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | KA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | KB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | KC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | KD    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | L     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | LA    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | LB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | LC    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | LD    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | M     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | MA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | MB    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | MC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | MD    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | N     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | NA    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | NB    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | NC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | ND    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | O     | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | OA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | OB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | OC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | OD    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | P     | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | PA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | PB    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | PC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | PD    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | Q     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | QA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | QB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | QC    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | R     | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | RA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | RB    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | RC    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | S     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | SA    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | SB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | SC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | T     | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | TA    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | TB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | TC    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | U     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | UA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | UB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | UC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | V     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | VA    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | VB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | VC    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | W     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | WA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | WB    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | WC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | X     | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | XA    | 115/125 (92%) | 115 (100%) | 0        | 100         | 100 |
| 1   | XB    | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | XC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | Y     | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |
| 1   | YA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | YB    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | YC    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | Z     | 113/125 (90%) | 112 (99%)  | 1 (1%)   | 75          | 86  |
| 1   | ZA    | 113/125 (90%) | 113 (100%) | 0        | 100         | 100 |
| 1   | ZB    | 116/125 (93%) | 116 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 1   | ZC    | 113/125 (90%)     | 113 (100%)   | 0        | 100         | 100 |
| All | All   | 13656/15000 (91%) | 13644 (100%) | 12 (0%)  | 92          | 97  |

All (12) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 58  | ARG  |
| 1   | P     | 58  | ARG  |
| 1   | Z     | 58  | ARG  |
| 1   | JA    | 58  | ARG  |
| 1   | TA    | 58  | ARG  |
| 1   | DB    | 58  | ARG  |
| 1   | NB    | 58  | ARG  |
| 1   | XB    | 58  | ARG  |
| 1   | HC    | 58  | ARG  |
| 1   | RC    | 58  | ARG  |
| 1   | BD    | 58  | ARG  |
| 1   | LD    | 58  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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.