



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:36 PM UTC

PDB ID : 8VKR / pdb\_00008vkr  
EMDB ID : EMD-43328  
Title : CW Flagellar Switch Complex with extra density - FliF, FliG, FliM, and FliN forming the C-ring from Salmonella  
Authors : Singh, P.K.; Iverson, T.M.  
Deposited on : 2024-01-09  
Resolution : 5.90 Å(reported)

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 : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

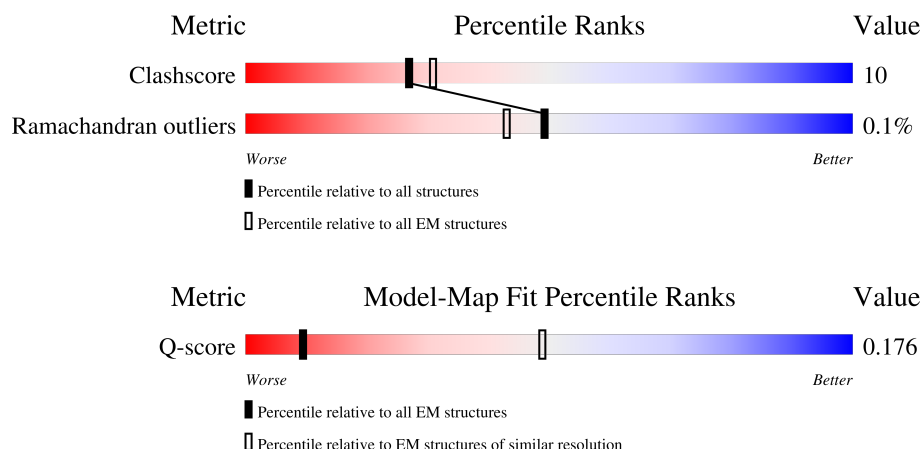
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.90 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Q-score               | -                           | 25397                       | 501 ( 5.40 - 6.40 )                                      |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                        |
|-----|-------|--------|---------------------------------------------------------|
| 1   | A     | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div> |
| 1   | BC    | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div> |
| 1   | BF    | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div> |
| 1   | DB    | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div> |
| 1   | DE    | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                    |     |
|-----|-------|--------|-------------------------------------------------------------------------------------|-----|
| 1   | F     | 560    |    | 92% |
| 1   | FA    | 560    |    | 92% |
| 1   | FD    | 560    |    | 92% |
| 1   | FG    | 560    |    | 92% |
| 1   | HC    | 560    |    | 92% |
| 1   | HF    | 560    |    | 92% |
| 1   | I     | 560    |    | 92% |
| 1   | JB    | 560    |    | 92% |
| 1   | JE    | 560    |    | 92% |
| 1   | LA    | 560    |    | 92% |
| 1   | LD    | 560    |   | 92% |
| 1   | LG    | 560    |  | 92% |
| 1   | NC    | 560    |  | 92% |
| 1   | NF    | 560    |  | 92% |
| 1   | PB    | 560    |  | 92% |
| 1   | PE    | 560    |  | 92% |
| 1   | RA    | 560    |  | 92% |
| 1   | RD    | 560    |  | 92% |
| 1   | RG    | 560    |  | 92% |
| 1   | S     | 560    |  | 92% |
| 1   | TC    | 560    |  | 92% |
| 1   | TF    | 560    |  | 92% |
| 1   | VB    | 560    |  | 92% |
| 1   | VE    | 560    |  | 92% |
| 1   | XA    | 560    |  | 92% |

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| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | XD    | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div>                |
| 1   | Z     | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div>                |
| 1   | ZC    | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div>                |
| 1   | ZF    | 560    | <div> <div>7%</div> <div>8%</div> <div>92%</div> </div>                |
| 2   | AA    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | AD    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |
| 2   | AG    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | B     | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | CC    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | CF    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | EB    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | EE    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | G     | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | GA    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |
| 2   | GD    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |
| 2   | GG    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | IC    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | IF    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | J     | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | KB    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |
| 2   | KE    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |
| 2   | MA    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |
| 2   | MD    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | MG    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div> |
| 2   | OC    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 2   | OF    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | QB    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>  |
| 2   | QE    | 331    | <div> <div>26%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>  |
| 2   | SA    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | SD    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | SG    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | T     | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | UC    | 331    | <div> <div>25%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>  |
| 2   | UF    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | WB    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | WE    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | YA    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 2   | YD    | 331    | <div> <div>25%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>  |
| 3   | BA    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | BD    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | BG    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | C     | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | DC    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | DF    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | FB    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | FE    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | HA    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | HD    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | HG    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | JC    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |

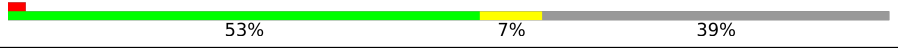
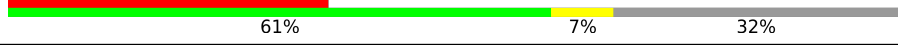
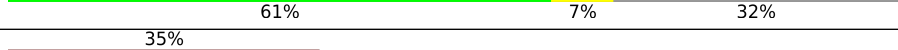
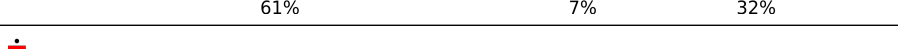
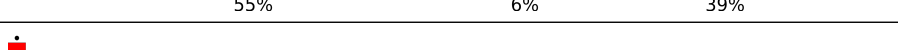
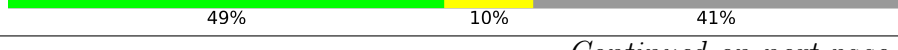
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| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 3   | JF    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | K     | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | LB    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | LE    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | M     | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | NA    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | ND    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | NG    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | PC    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | PF    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | RB    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | RE    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | TA    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | TD    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | TG    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | V     | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | VC    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | VF    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | XB    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | XE    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | ZA    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 3   | ZD    | 334    | <div> <div>23%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div> |
| 4   | AB    | 137    | <div> <div>36%</div> <div>63%</div> <div>5%</div> <div>32%</div> </div> |
| 4   | AC    | 137    | <div> <div>50%</div> <div>9%</div> <div>41%</div> </div>                |
| 4   | AE    | 137    | <div> <div>36%</div> <div>61%</div> <div>7%</div> <div>32%</div> </div> |

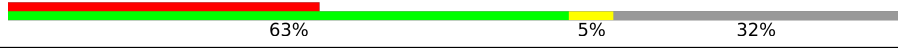
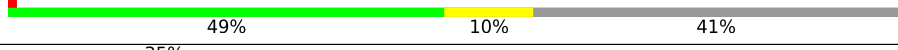
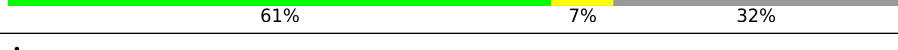
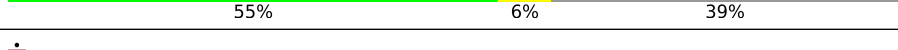
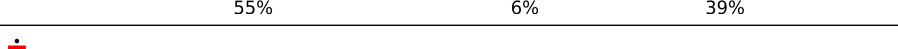
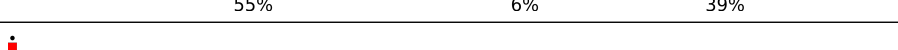
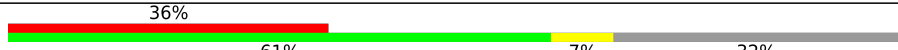
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | AF    | 137    |    |
| 4   | BB    | 137    |    |
| 4   | BE    | 137    |    |
| 4   | CA    | 137    |    |
| 4   | CB    | 137    |    |
| 4   | CD    | 137    |    |
| 4   | CE    | 137    |    |
| 4   | CG    | 137    |    |
| 4   | D     | 137    |    |
| 4   | DA    | 137    |    |
| 4   | DD    | 137    |    |
| 4   | DG    | 137    |  |
| 4   | E     | 137    |  |
| 4   | EA    | 137    |  |
| 4   | EC    | 137    |  |
| 4   | ED    | 137    |  |
| 4   | EF    | 137    |  |
| 4   | EG    | 137    |  |
| 4   | FC    | 137    |  |
| 4   | FF    | 137    |  |
| 4   | GB    | 137    |  |
| 4   | GC    | 137    |  |
| 4   | GE    | 137    |  |
| 4   | GF    | 137    |  |
| 4   | H     | 137    |  |

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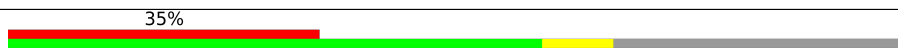
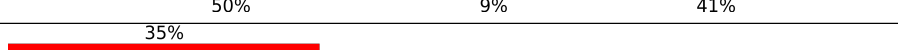
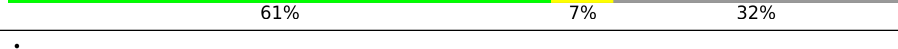
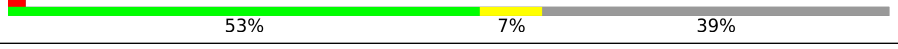
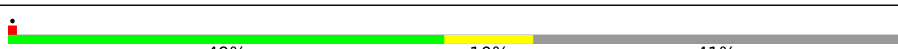
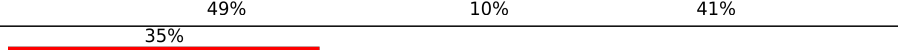
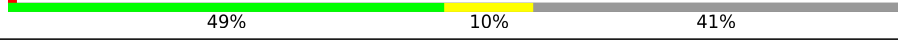
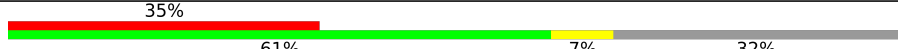
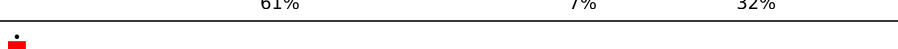
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | HB    | 137    |    |
| 4   | HE    | 137    |    |
| 4   | IA    | 137    |    |
| 4   | IB    | 137    |    |
| 4   | ID    | 137    |    |
| 4   | IE    | 137    |    |
| 4   | IG    | 137    |    |
| 4   | JA    | 137    |    |
| 4   | JD    | 137    |    |
| 4   | JG    | 137    |    |
| 4   | KA    | 137    |    |
| 4   | KC    | 137    |  |
| 4   | KD    | 137    |  |
| 4   | KF    | 137    |  |
| 4   | KG    | 137    |  |
| 4   | L     | 137    |  |
| 4   | LC    | 137    |  |
| 4   | LF    | 137    |  |
| 4   | MB    | 137    |  |
| 4   | MC    | 137    |  |
| 4   | ME    | 137    |  |
| 4   | MF    | 137    |  |
| 4   | N     | 137    |  |
| 4   | NB    | 137    |  |
| 4   | NE    | 137    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | O     | 137    |    |
| 4   | OA    | 137    |    |
| 4   | OB    | 137    |    |
| 4   | OD    | 137    |    |
| 4   | OE    | 137    |    |
| 4   | OG    | 137    |    |
| 4   | P     | 137    |    |
| 4   | PA    | 137    |    |
| 4   | PD    | 137    |    |
| 4   | PG    | 137    |    |
| 4   | Q     | 137    |    |
| 4   | QA    | 137    |    |
| 4   | QC    | 137    |   |
| 4   | QD    | 137    |  |
| 4   | QF    | 137    |  |
| 4   | QG    | 137    |  |
| 4   | R     | 137    |  |
| 4   | RC    | 137    |  |
| 4   | RF    | 137    |  |
| 4   | SB    | 137    |  |
| 4   | SC    | 137    |  |
| 4   | SE    | 137    |  |
| 4   | SF    | 137    |  |
| 4   | TB    | 137    |  |
| 4   | TE    | 137    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | UA    | 137    |                  |
| 4   | UB    | 137    |                  |
| 4   | UD    | 137    |                  |
| 4   | UE    | 137    |                  |
| 4   | UG    | 137    |                  |
| 4   | VA    | 137    |                  |
| 4   | VD    | 137    |                  |
| 4   | VG    | 137    |                  |
| 4   | W     | 137    |                  |
| 4   | WA    | 137    |                  |
| 4   | WC    | 137    |                  |
| 4   | WD    | 137    |                  |
| 4   | WF    | 137    |                  |
| 4   | WG    | 137    |                  |
| 4   | X     | 137    |                  |
| 4   | XC    | 137    |                  |
| 4   | XF    | 137    |                  |
| 4   | Y     | 137    |                  |
| 4   | YB    | 137    |                  |
| 4   | YC    | 137    |                  |
| 4   | YE    | 137    |                  |
| 4   | YF    | 137    |                  |
| 4   | ZB    | 137    |                  |
| 4   | ZE    | 137    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 152898 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 Flagellar M-ring protein.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | F     | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | A     | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | I     | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | S     | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | Z     | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | FA    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | LA    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | RA    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | XA    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | DB    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | JB    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | PB    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | VB    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | BC    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | HC    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | NC    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | TC    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | ZC    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | FD    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | LD    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | RD    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | XD    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | DE    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | JE    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | PE    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | VE    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | BF    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | HF    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | NF    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | TF    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | ZF    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | FG    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | LG    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |
| 1   | RG    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 234   | 140 | 47 | 47 |         |       |

- Molecule 2 is a protein called Flagellar motor switch protein FliG.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | G     | 319      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1579  | 941 | 319 | 319 |         |       |
| 2   | B     | 319      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1579  | 941 | 319 | 319 |         |       |

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| Mol | Chain | Residues | Atoms         |          |          |          | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|-------|
| 2   | J     | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | T     | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | AA    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | GA    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | MA    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | SA    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | YA    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | EB    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | KB    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | QB    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | WB    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | CC    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | IC    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | OC    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | UC    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | AD    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | GD    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | MD    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | SD    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | YD    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | EE    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |          |          |          | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|-------|
| 2   | KE    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | QE    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | WE    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | CF    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | IF    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | OF    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | UF    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | AG    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | GG    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | MG    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |
| 2   | SG    | 319      | Total<br>1579 | C<br>941 | N<br>319 | O<br>319 | 0       | 0     |

- Molecule 3 is a protein called Flagellar motor switch protein FliM.

| Mol | Chain | Residues | Atoms         |          |          |          | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|-------|
| 3   | M     | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |
| 3   | C     | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |
| 3   | K     | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |
| 3   | V     | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |
| 3   | BA    | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |
| 3   | HA    | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |
| 3   | NA    | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |
| 3   | TA    | 287      | Total<br>1420 | C<br>846 | N<br>287 | O<br>287 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | ZA    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | FB    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | LB    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | RB    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | XB    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | DC    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | JC    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | PC    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | VC    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | BD    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | HD    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | ND    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | TD    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | ZD    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | FE    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | LE    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | RE    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | XE    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | DF    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | JF    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | PF    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | VF    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | BG    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | HG    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | NG    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |
| 3   | TG    | 287      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1420  | 846 | 287 | 287 |         |       |

- Molecule 4 is a protein called Flagellar motor switch protein FliN.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | N     | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | P     | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | Q     | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | D     | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | E     | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | H     | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | L     | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | O     | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | R     | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | W     | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | X     | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | Y     | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | CA    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | DA    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | EA    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | IA    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | JA    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | KA    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | OA    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | PA    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | QA    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | UA    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | VA    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | WA    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | AB    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | BB    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | CB    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | GB    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | HB    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | IB    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | MB    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | NB    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | OB    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | SB    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | TB    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | UB    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | YB    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | ZB    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | AC    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | EC    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | FC    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | GC    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | KC    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | LC    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | MC    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | QC    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | RC    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | SC    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | WC    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | XC    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | YC    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | CD    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | DD    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | ED    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | ID    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | JD    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | KD    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | OD    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | PD    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | QD    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | UD    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | VD    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | WD    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | AE    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | BE    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | CE    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | GE    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | HE    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | IE    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | ME    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | NE    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | OE    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | SE    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | TE    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | UE    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | YE    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | ZE    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | AF    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | EF    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | FF    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | GF    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | KF    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | LF    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | MF    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | QF    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | RF    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | SF    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | WF    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | XF    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | YF    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | CG    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | DG    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | EG    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | IG    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | JG    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | KG    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | OG    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | PG    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |

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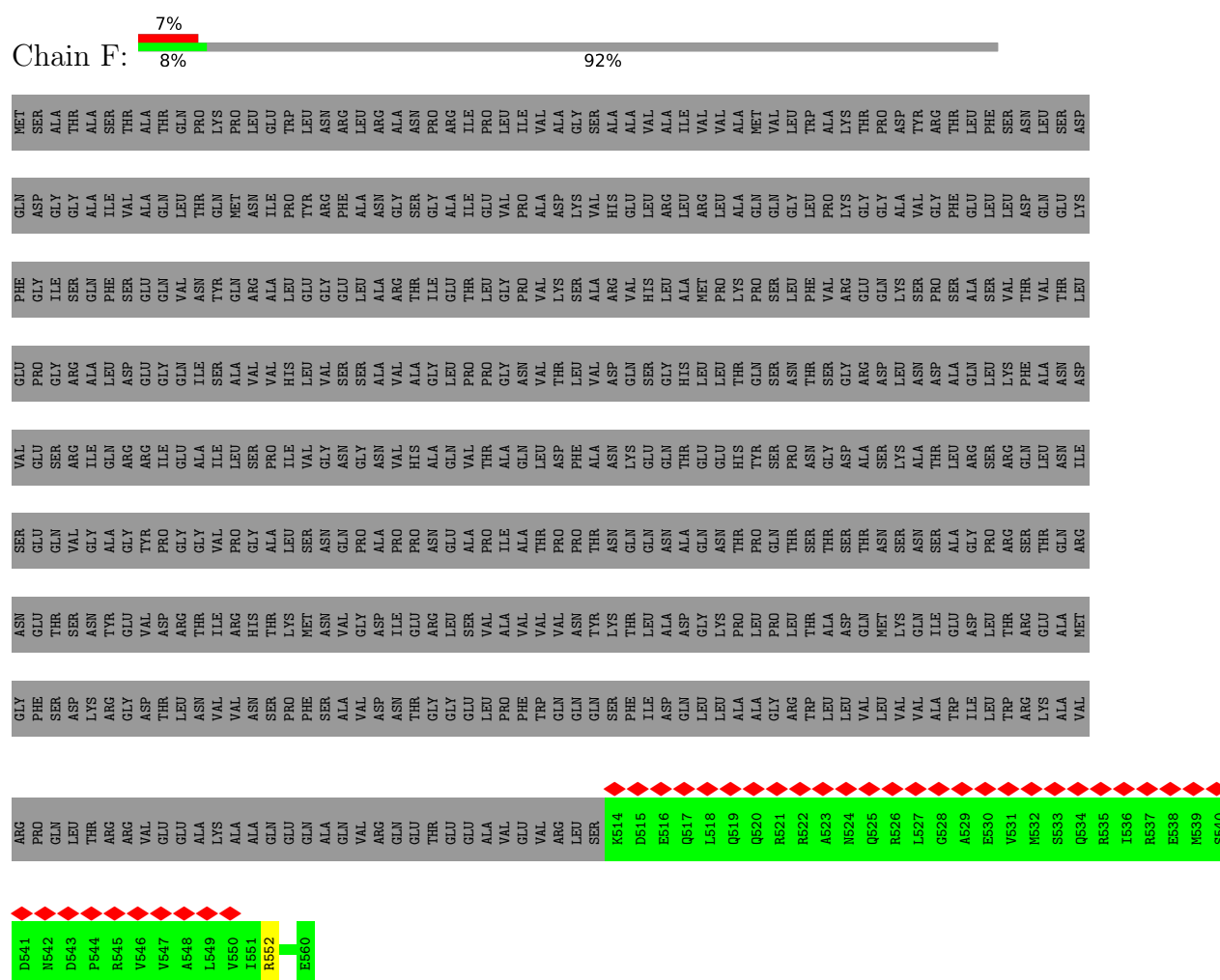
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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | QG    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |
| 4   | UG    | 93       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 456   | 270 | 93 | 93 |         |       |
| 4   | VG    | 83       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 242 | 83 | 84 |         |       |
| 4   | WG    | 81       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 399   | 236 | 81 | 82 |         |       |

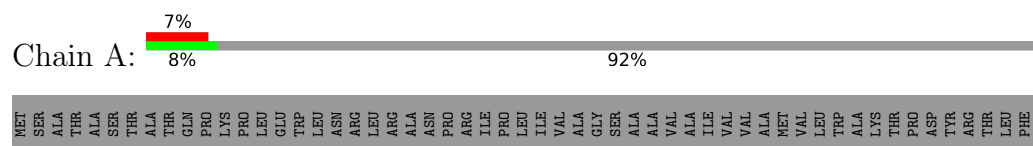
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Flagellar M-ring protein



#### • Molecule 1: Flagellar M-ring protein

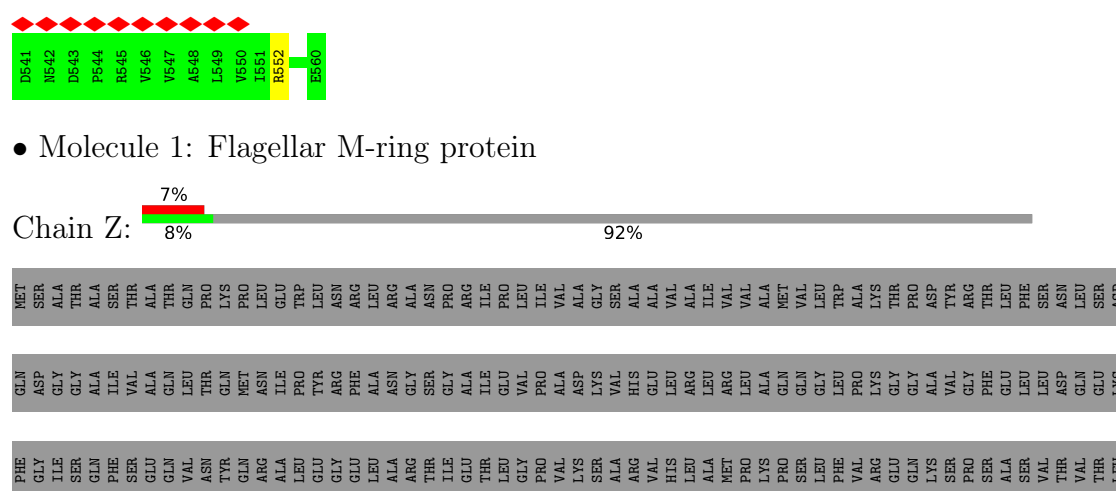
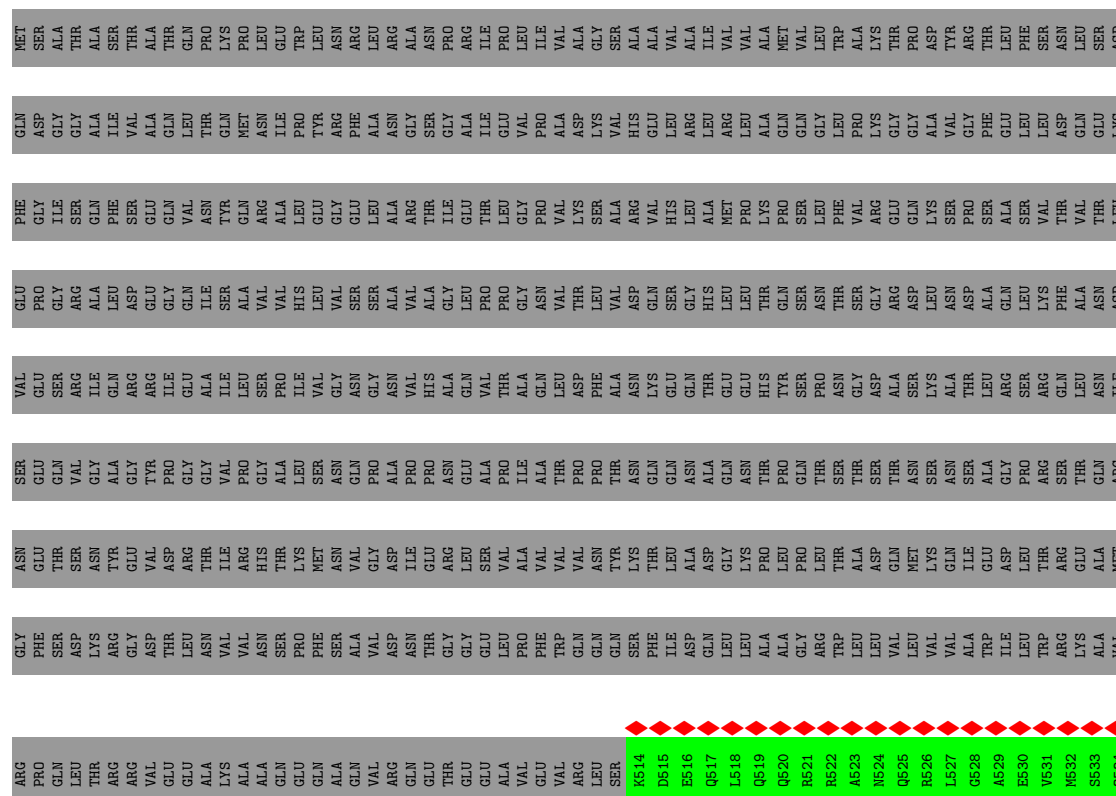


|      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D541 | N542 | D543 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain I:  7% 8% 92%



- Molecule 1: Flagellar M-ring protein



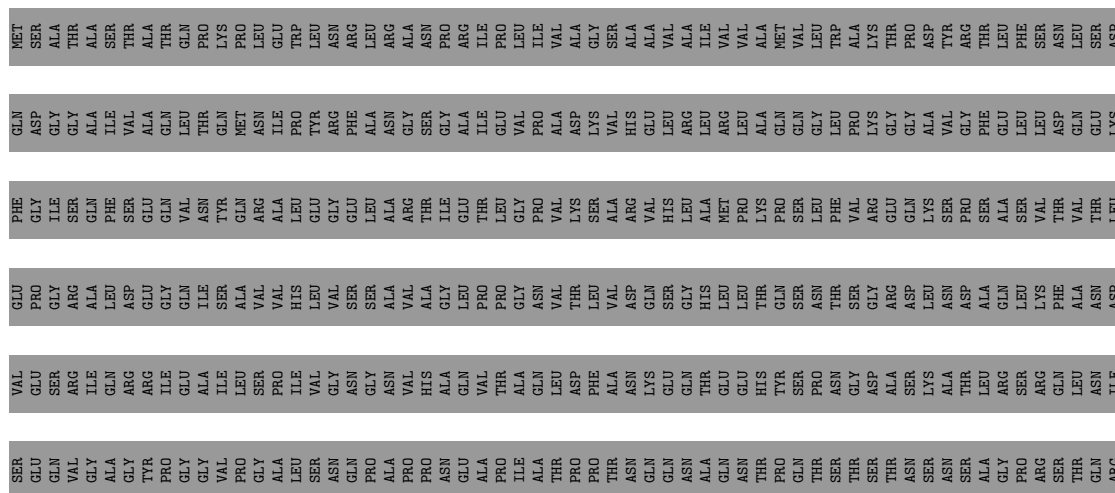
- Molecule 1: Flagellar M-ring protein







Chain LA:  7% 8% 92%



|      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D641 | D542 | D643 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 | ARG | PRO | GLN | LEU | THR | ARG | ARG | VAL | GLU | GLU | ALA | LYS | ALA | ALA | ALA | GLN | GLN | GLN | VAL | ARG | GLN | GLU | THR | GLU | GLU | ALA | VAL | VAL | ARG | VAL | GLU | VAL | ARG | LEU | SER | K514 | D515 | E516 | Q517 | L518 | Q519 | Q520 | R521 | R522 | A523 | N524 | Q525 | R526 | L527 | G528 | A529 | E530 | V531 | M532 | S533 | Q534 | R535 | I536 | R537 | E538 | M539 | S540 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain XA: 

|      |     |     |     |     |     |     |     |     |     |     |     |     |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| D641 | ARG | GLY | ASN | SER | VAL | GLU | PRO | PHE | GLN | GLY | ASP | MET |
| N542 | GLN | SER | THR | GLU | GLY | GLU | GLU | THR | GLN | ILE | GLY | SER |
| D643 | LEU | ASP | ASN | VAL | GLY | VAL | GLY | VAL | ARG | ALA | GLY | THR |
| P544 | THR | LYS | ASN | THR | ALA | ALA | ALA | GLY | GLN | PHE | ILE | SER |
| R645 | ARG | ARG | GLY | GLU | GLY | THR | GLY | THR | ARG | SER | VAL | THR |
| V546 | VAL | ASP | VAL | VAL | TYR | ARG | ARG | GLU | GLU | GLY | ALA | ALA |
| V547 | GLU | THR | GLY | GLY | GLY | GLY | ILE | GLN | GLN | VAL | LEU | GLN |
| A548 | GLU | LEU | ARG | GLY | GLY | GLY | ALA | ILE | ILE | ASN | THR | PRO |
| L549 | ALA | ASN | THR | THR | VAL | GLY | GLY | ALA | SER | TYR | GLN | LYS |
| V550 | LYS | VAL | ARG | PRO | LEU | ALA | ALA | ILE | GLN | GLN | MET | PRO |
| I551 | ALA | ASN | HIS | GLY | GLY | SER | VAL | ARG | ASN | ASN | LEU | GLY |
| R552 | GLN | SER | THR | THR | ALA | ALA | ILE | ILE | ALA | ALA | ILE | TRP |
| E553 | GLU | PHE | MET | ASN | VAL | VAL | VAL | SER | VAL | GLY | TYR | ASN |
| E554 | ALA | SER | ASN | GLN | GLY | ASN | GLY | GLY | GLY | GLY | ARG | ASN |
| E555 | GLN | ALA | VAL | VAL | ALA | GLN | GLN | GLU | LEU | LEU | PHE | ARG |
| E556 | VAL | VAL | GLY | GLY | ASP | PRO | THR | THR | VAL | VAL | ALA | VAL |
| E557 | ARG | GLN | VAL | VAL | ASN | PRO | PRO | PRO | LYS | ASP | ALA | ALA |
| E558 | LEU | GLN | THR | THR | THR | THR | THR | THR | ALA | VAL | SER | SER |
| E559 | SER | SER | LYS | THR | GLN | GLN | GLN | GLN | ASN | VAL | HIS | ALA |
| E560 | THR | PHE | LEU | LEU | THR | GLN | GLY | SER | ASN | GLY | LEU | VAL |
| E561 | THR | ILE | ASP | ALA | GLY | GLY | GLY | THR | GLY | ARG | ALA | GLY |
| E562 | THR | GLN | ASP | ALA | ASN | GLN | GLN | THR | GLY | ALA | ILE | ILE |
| E563 | LEU | LEU | GLY | GLY | GLN | GLU | GLU | MET | ARG | VAL | ARG | VAL |
| E564 | ALA | LEU | LYS | PRO | ASN | THR | LYS | THR | PRO | ALA | PRO | ALA |
| E565 | VAL | ALA | PRO | LEU | THR | THR | HIS | THR | LYS | ALA | ALA | VAL |
| E566 | THR | THR | THR | THR | THR | GLN | THR | THR | PRO | GLN | GLN | MET |
| E567 | THR | GLY | PRO | GLN | THR | SER | SER | SER | SER | GLN | GLN | VAL |
| E568 | THR | ARG | THR | THR | THR | THR | THR | THR | THR | GLY | GLY | THR |
| E569 | THR | THR | THR | THR | THR | THR | THR | THR | THR | GLY | GLY | PRO |
| E570 | THR | THR | THR | THR | THR | THR | THR | THR | THR | ALA | ASP | TYR |
| E571 | THR | THR | THR | THR | THR | THR | THR | THR | THR | GLY | VAL | THR |
| E572 | THR | THR | THR | THR | THR | THR | THR | THR | THR | PHE | PHE | THR |
| E573 | THR | THR | THR | THR | THR | THR | THR | THR | THR | ALA | GLU | LEU |
| E574 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E575 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E576 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E577 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E578 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E579 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E580 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E581 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E582 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E583 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E584 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E585 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E586 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E587 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E588 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E589 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E590 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E591 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E592 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E593 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E594 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E595 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E596 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E597 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E598 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E599 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
| E600 | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |

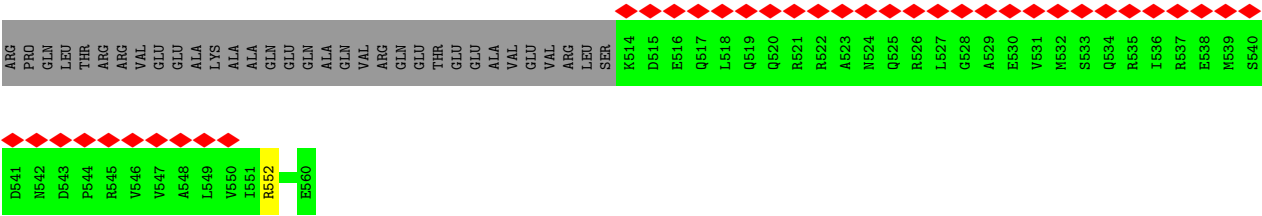
Chain DB:  7% 8% 92%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | ALA | ALA | THR | THR | SER | THR | ALA | GLN | PRO | LYS | LEU | GLY | TRP | ASN | ARG | LEU | ARG | ALA | ASN | PRO | ARG | ILE | PRO | LEU | ILE | VAL | ALA | GLY | SER | ALA | ALA | VAL | ALA | ALA | ILE | VAL | VAL | VAL | MET | VAL | VAL | LEU | TRP | TYR | ARG | THR | LEU | PHE | SER | ASN | LEU | SER | ASP | PRO | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

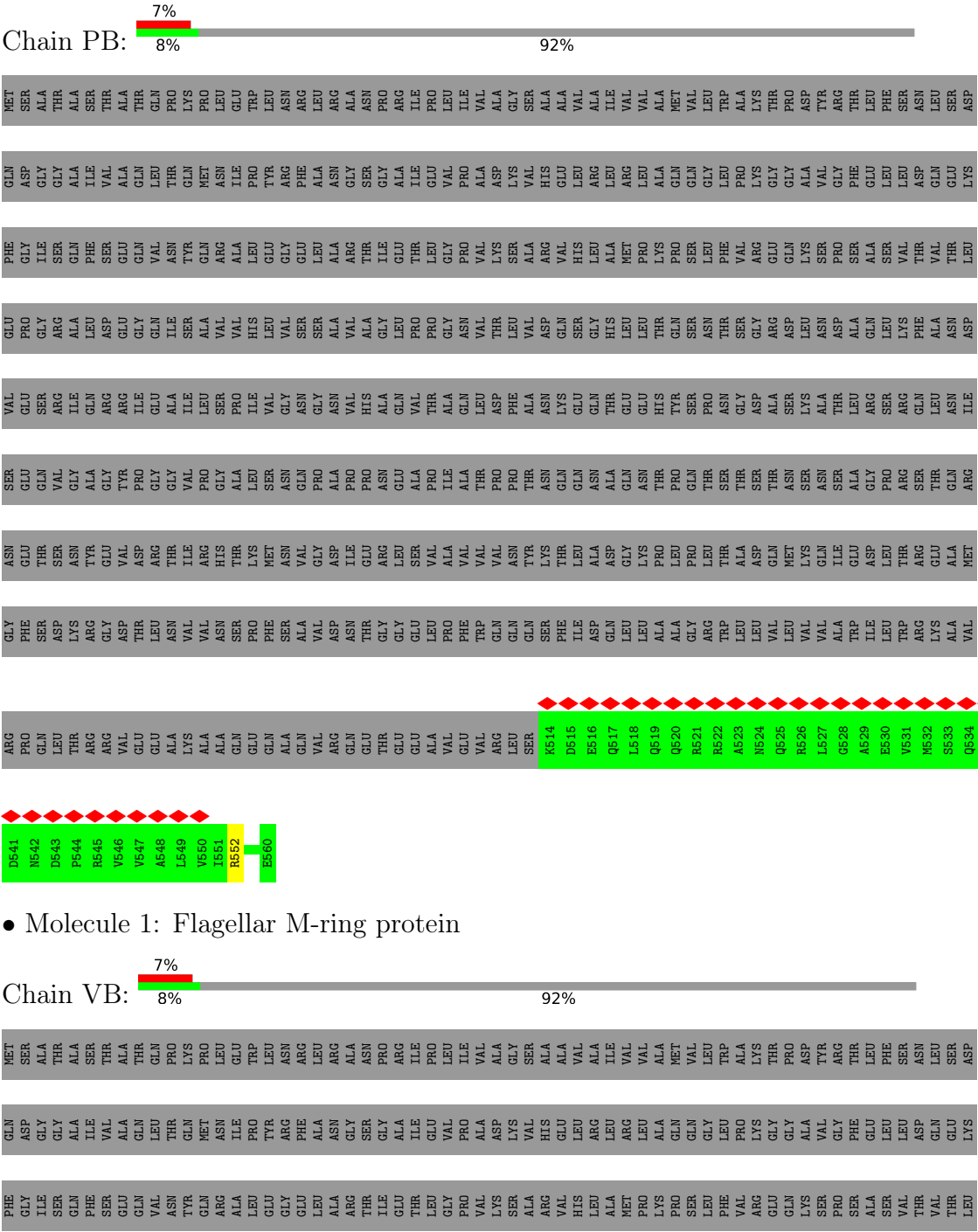
|      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D541 | N542 | D543 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain JB: 

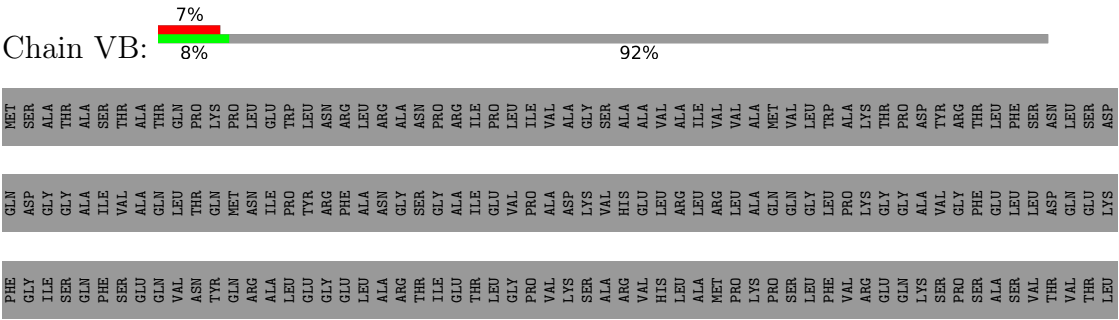




• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



|      |     |      |
|------|-----|------|
| D541 | ARG | ARG  |
| N542 | PRO | GLN  |
| D543 | LEU | THR  |
| P544 | THR | ARG  |
| R545 | ARG | VAL  |
| V546 | VAL | GLU  |
| A547 | GLU | LYS  |
| L549 | ALA | ALA  |
| V550 | GLN | GLN  |
| I551 | GLU | GLN  |
| R552 | GLU | GLN  |
|      | ALA | VAL  |
|      | VAL | GLU  |
|      | VAL | VAL  |
|      | ARG | ARG  |
|      | LEU | LEU  |
|      | SER | K514 |
|      |     | D515 |
|      |     | E516 |
|      |     | Q517 |
|      |     | L518 |
|      |     | Q519 |
|      |     | Q520 |
|      |     | R521 |
|      |     | R522 |
|      |     | A523 |
|      |     | N524 |
|      |     | Q525 |
|      |     | R526 |
|      |     | L527 |
|      |     | G528 |
|      |     | A529 |
|      |     | E530 |
|      |     | V531 |
|      |     | M532 |
|      |     | S533 |
|      |     | Q534 |
|      |     | R535 |
|      |     | I536 |
|      |     | R537 |
|      |     | E538 |
|      |     | M539 |
|      |     | S540 |

Chain BC: 

|      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D641 | N542 | D643 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | T551 | R552 | E560 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain HC: 



|      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D641 | D542 | D643 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 | ARG | PRO | GLN | LEU | THR | ARG | ARG | VAL | GLU | GLU | ALA | LYS | ALA | ALA | ALA | GLN | GLN | GLN | VAL | ARG | GLN | GLU | THR | GLU | GLU | ALA | VAL | VAL | ARG | VAL | GLU | VAL | ARG | LEU | SER | K514 | D515 | E516 | Q517 | L518 | Q519 | Q520 | R521 | R522 | A523 | N524 | Q525 | R526 | L527 | G528 | A529 | E530 | V531 | M532 | S533 | Q534 | R535 | I536 | R537 | E538 | M539 | S540 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain TC: 

[illegible]

Chain ZC: 

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | ALA | ALA | THR | THR | SER | THR | ALA | GLN | PRO | LYS | LEU | GLY | TRP | ASN | ARG | LEU | ARG | ALA | ASN | PRO | ARG | ILE | LEU | ILE | VAL | ALA | GLY | SER | ALA | ALA | VAL | ALA | ALA | ILE | VAL | VAL | VAL | MET | VAL | VAL | LEU | TRP | TYR | ARG | THR | LEU | PHE | SER | ASN | LEU | SER | ASP | PRO | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

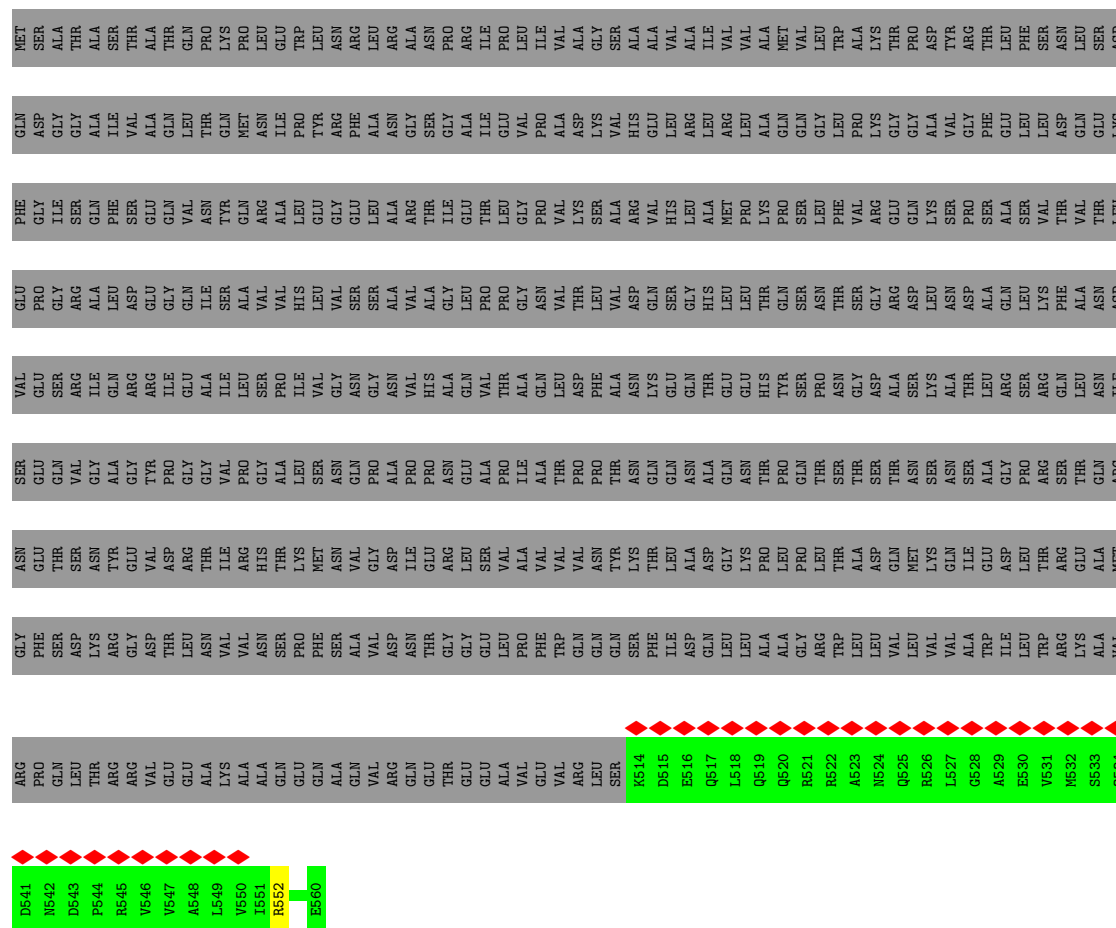


|      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D541 | N542 | D543 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|

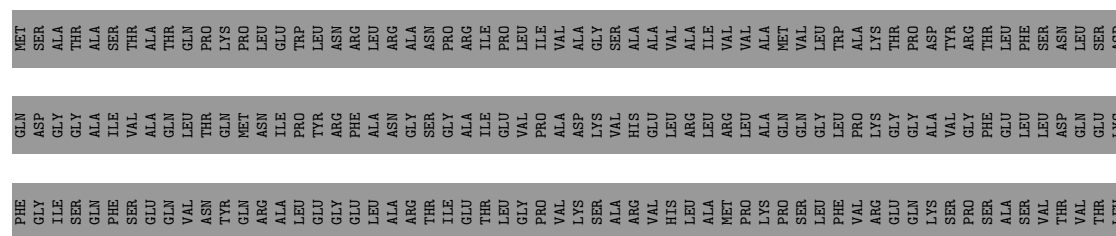
Chain FD: 



- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein





Chain DE: 



|      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D541 | N542 | D543 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain PE: 

|      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D541 | N542 | D543 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain VE: 

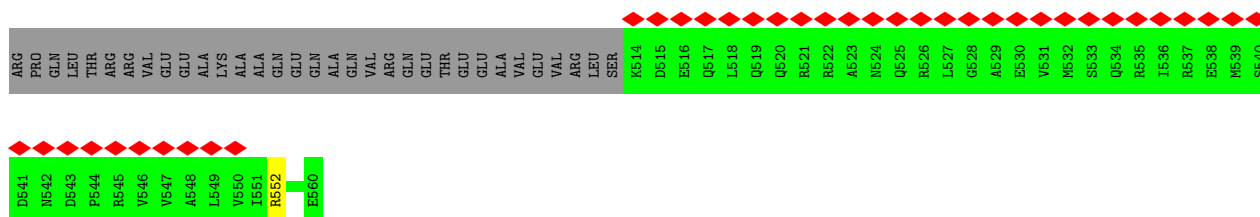
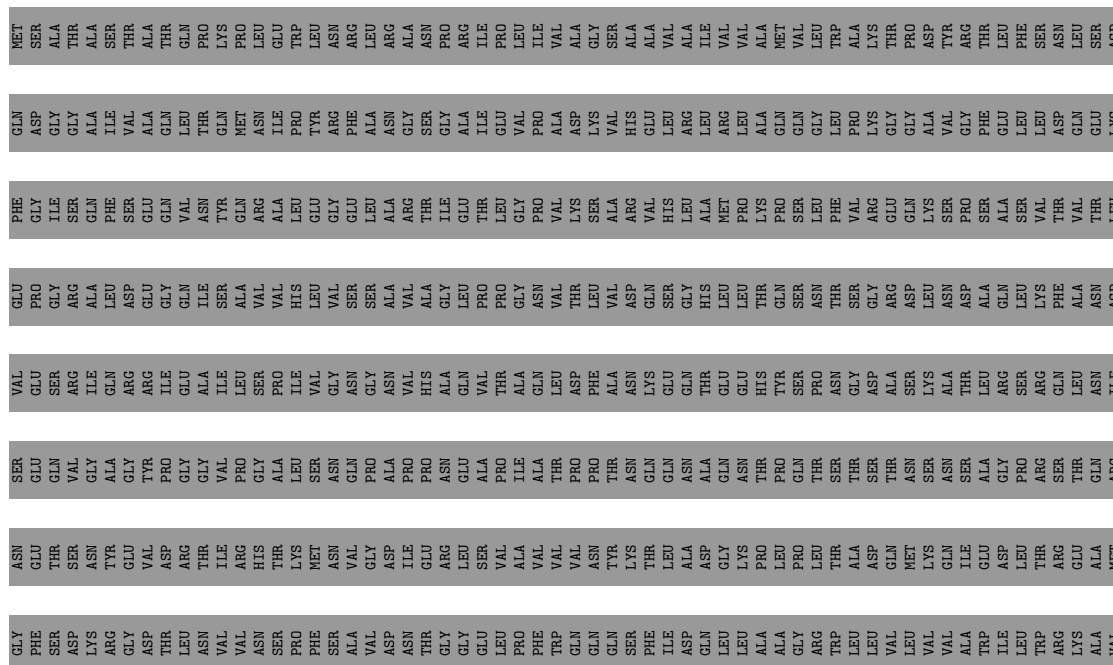
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | THR | ALA | SER | THR | ALA | GLN | PRO | LYS | PRO | LEU | GLU | TRP | LEU | ASN | ARG | LEU | ARG | ALA | ASN | PRO | ARG | ILE | PRO | LEU | ILE | VAL | ALA | GLY | SER | ALA | ALA | VAL | VAL | ALA | ILE | VAL | VAL | VAL | ALA | VAL | MET | VAL | VAL | LEU | TRP | LEU | ALA | ALA | LYS | THR | PRO | ASP | TYR | ARG | THR | LEU | PHE | SER | ASN | LEU | LEU | SER | ASN | GLN | PRO | LEU | GLU | TRP | LEU | ASN | ARG | LEU | ARG | ALA | GLN | PRO | LYS | PRO | LEU | GLU | TRP | LEU | ASN | ARG | LEU | THR | ALA | SER | THR | ALA | THR | ALA | SER | ALA | MET |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

Diagram illustrating a 16-bit bus structure. The bus is divided into 16 segments, labeled D541, N542, D543, P544, R545, V546, V547, A548, L549, V550, I551, R552, and E560. The segments are connected sequentially, with a green arrow indicating a connection from the 16th segment (E560) to the 15th segment (R552).

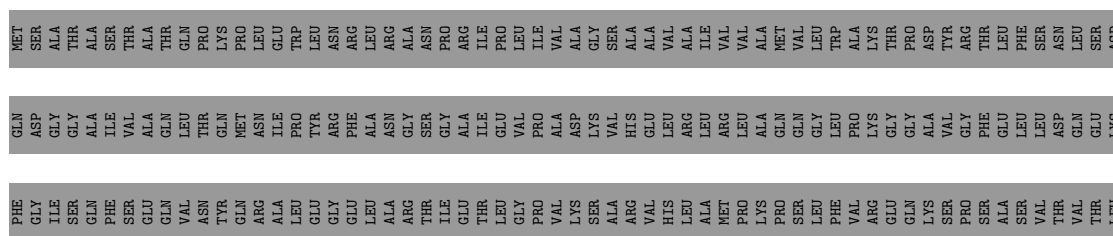
Chain BF: 

[illegible]

- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein



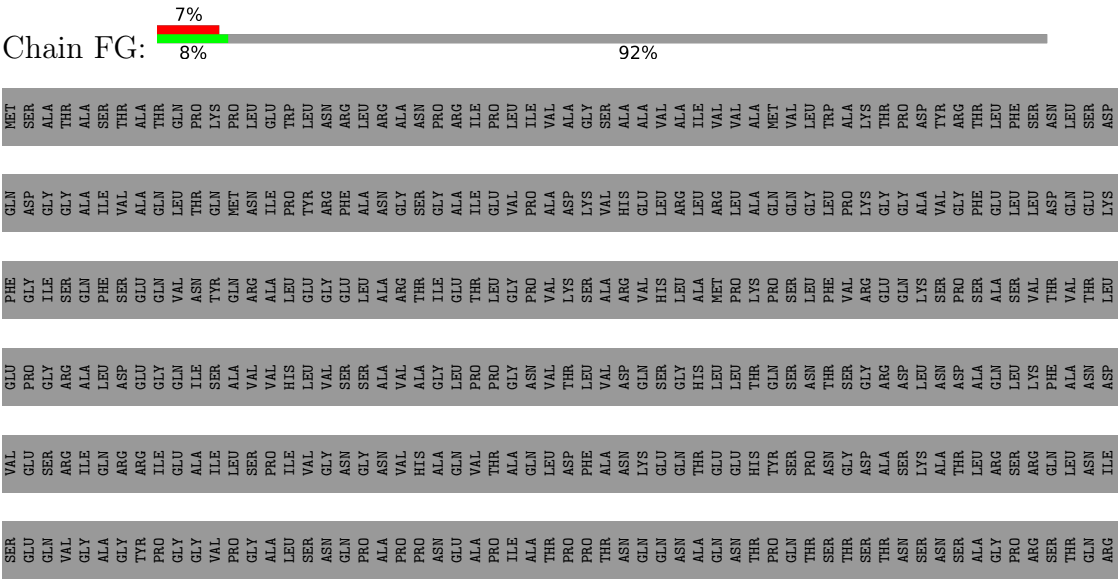




● Molecule 1: Flagellar M-ring protein



● Molecule 1: Flagellar M-ring protein



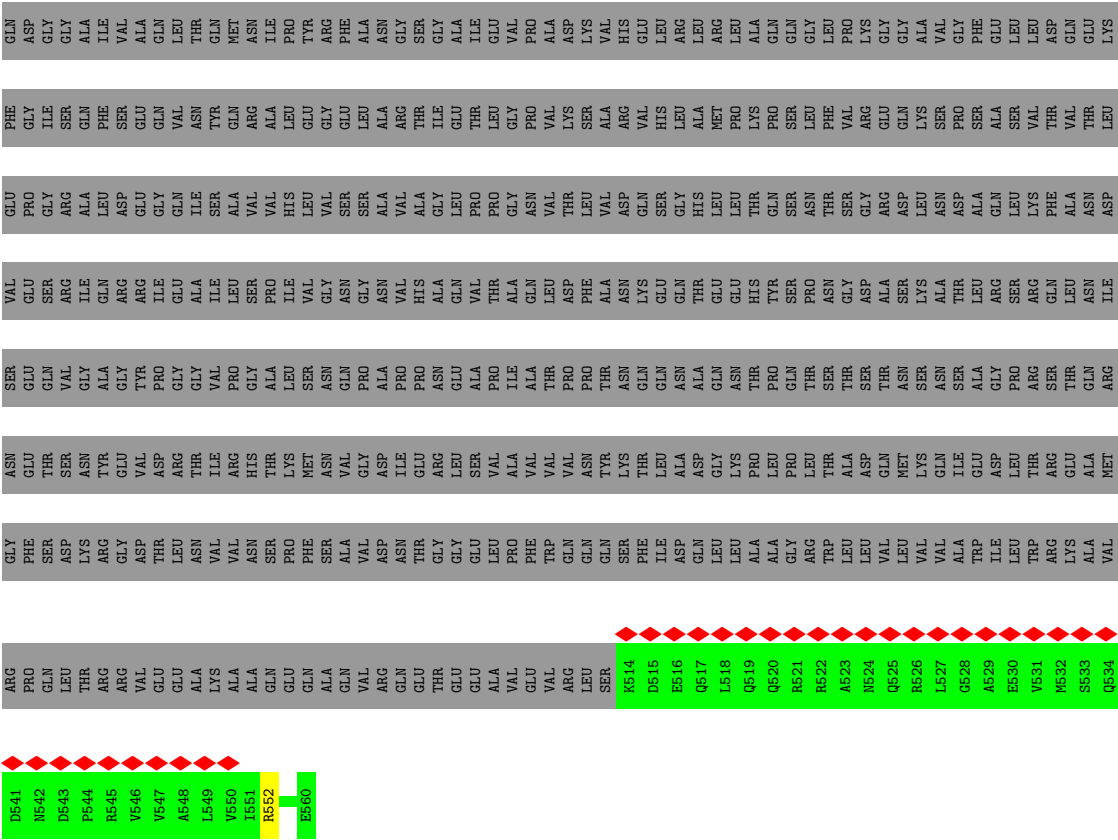
|      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D641 | D542 | D643 | P544 | R545 | V546 | V547 | A548 | L549 | V550 | I551 | R552 | E560 | ARG | PRO | GLN | LEU | THR | ARG | ARG | VAL | GLU | GLU | ALA | LYS | ALA | ALA | ALA | GLN | GLN | GLN | VAL | ARG | GLN | GLU | THR | GLU | GLU | ALA | VAL | VAL | ARG | VAL | GLU | VAL | ARG | LEU | SER | K514 | D515 | E516 | Q517 | L518 | Q519 | Q520 | R521 | R522 | A523 | N524 | Q525 | R526 | L527 | G528 | A529 | E530 | V531 | M532 | S533 | Q534 | R535 | I536 | R537 | E538 | M539 | S540 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

Chain LG:  7% 8% 92%

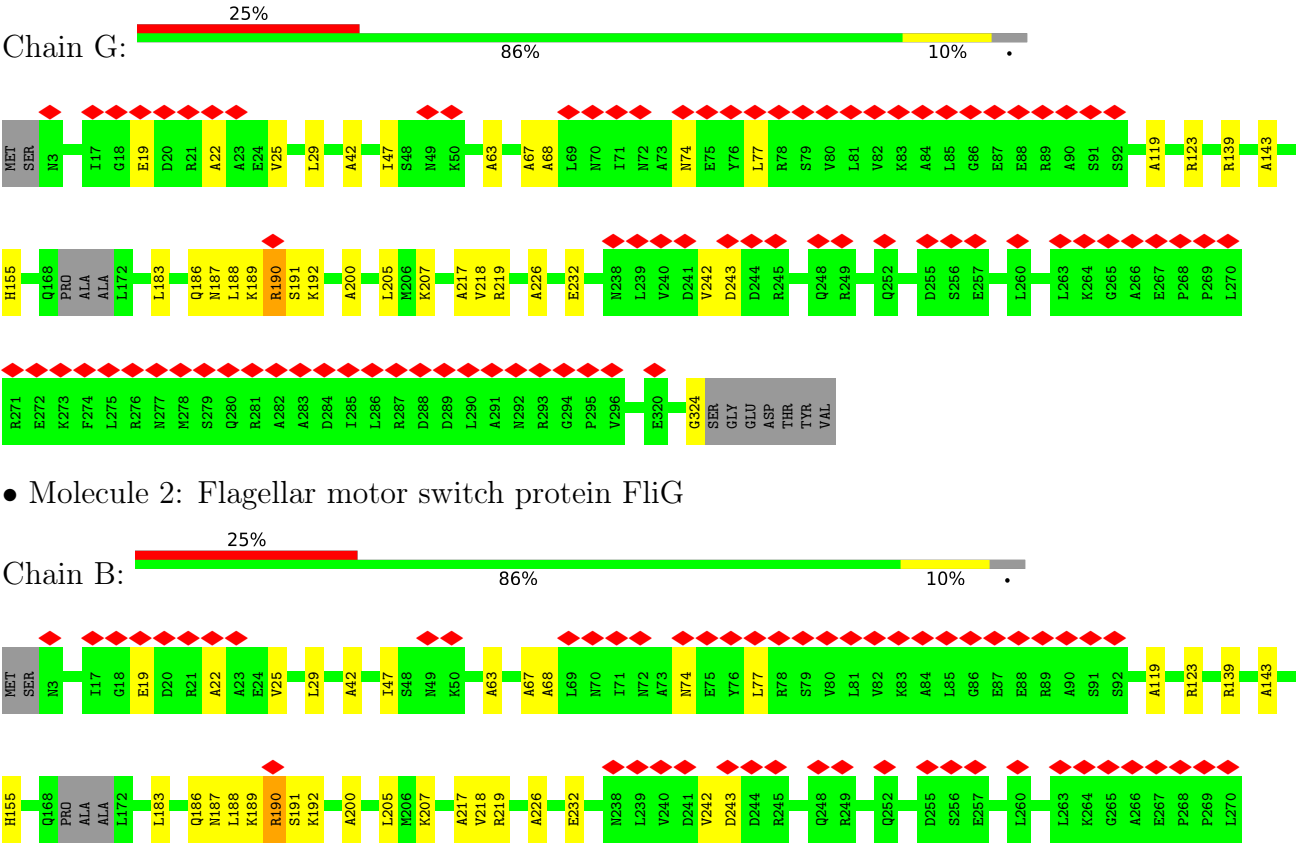
|      |     |     |     |     |     |     |     |     |     |     |     |     |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| D641 | ARG | GLY | ASN | SER | VAL | GLU | PRO | PHE | GLN | GLY | ASP | MET |
| N542 | GLN | SER | THR | GLU | GLY | GLU | GLU | THR | ILE | GLN | GLY | SER |
| D643 | LEU | ASP | ASN | VAL | GLY | VAL | GLY | GLY | ARG | ALA | GLY | THR |
| P544 | THR | LYS | ASN | THR | ALA | ALA | ALA | ALA | GLN | PHE | ILE | SER |
| R645 | ARG | ARG | GLY | GLU | GLY | THR | GLY | GLY | ARG | SER | VAL | THR |
| V546 | VAL | ASP | VAL | THR | TYR | ARG | GLU | GLU | GLU | GLY | ALA | ALA |
| V547 | GLU | THR | GLY | ARG | PRO | GLY | GLN | VAL | GLN | VAL | LEU | GLN |
| A548 | ALA | ASN | THR | THR | GLY | VAL | ILE | ALA | ILE | ASN | THR | PRO |
| L549 | LYS | VAL | ILE | ARG | PRO | LEU | ALA | SER | GLN | TYR | GLN | LYS |
| V550 | ALA | VAL | ARG | PRO | LEU | LEU | ALA | GLN | GLN | MET | PRO | PRO |
| I551 | ALA | ASN | SER | THR | HIS | VAL | SER | ARG | ASN | ASN | LEU | GLU |
| R552 | GLN | SER | THR | THR | ALA | VAL | ILE | PRO | ILE | ILE | TRP | LEU |
|      | GLY | PHE | MET | ASN | VAL | GLY | VAL | GLY | GLY | GLY | TYR | LEU |
| E560 | ALA | SER | ASN | ASN | GLY | ASN | SER | GLY | GLY | ARG | ASN | ASN |
|      | GLN | ALA | VAL | GLN | ASN | SER | SER | GLU | GLU | PHE | LEU | ARG |
|      | VAL | VAL | GLY | PRO | GLY | SER | GLY | LEU | ALA | ALA | ILE | PRO |
|      | ARG | ASP | ALA | ALA | ASN | ALA | VAL | THR | PRO | THR | GLU | ILE |
|      | GLN | ASN | ILE | PRO | VAL | VAL | VAL | ARG | GLY | GLY | ALA | ALA |
|      | GLU | THR | GLU | PRO | HIS | ALA | GLY | THR | SER | ASN | SER | ASN |
|      | THR | GLY | ARG | ASN | ALA | ALA | GLY | ILE | GLY | PRO | PRO | PRO |
|      | GLU | GLY | LEU | GLU | GLN | LEU | LEU | GLU | VAL | ALA | VAL | VAL |
|      | GLU | GLU | SER | ALA | VAL | THR | ALA | THR | VAL | VAL | ALA | ALA |
|      | VAL | PHE | VAL | VAL | VAL | GLN | ASN | PRO | GLY | LEU | VAL | VAL |
|      | VAL | THR | VAL | VAL | LEU | THR | ASN | THR | GLY | ALA | ALA | ALA |
|      | ARG | GLN | VAL | VAL | ASN | PRO | ASP | PRO | LYS | ASP | ASP | GLY |
|      | LEU | GLN | ASN | ASN | THR | THR | ALA | THR | VAL | VAL | VAL | SER |
|      | SER | SER | LYS | THR | GLN | GLN | LYS | GLN | ASN | ARG | HIS | SER |
|      |     | PHE | THR | THR | THR | LEU | GLN | THR | VAL | VAL | GLY | ALA |
|      |     | ILE | LEU | LEU | ALA | ASN | GLN | SER | GLY | GLY | LEU | ALA |
|      |     | ASP | ALA | ALA | ASN | GLN | GLN | THR | HIS | THR | ARG | ALA |
|      |     | GLN | ASP | ASP | THR | THR | GLY | GLY | VAL | VAL | PRO | ALA |
|      |     | LEU | GLN | SER | THR | THR | ASN | PHE | THR | THR | LEU | THR |
|      |     | VAL | MET | THR | ASN | THR | THR | GLY | GLY | GLY | LYS | LYS |
|      |     | VAL | LYS | LYS | ASN | VAL | ASN | ALA | ASP | GLY | GLY | THR |
|      |     | VAL | GLN | ASN | THR | THR | ASN | SER | ASP | GLY | GLY | PRO |
|      |     | ALA | ILE | ILE | ASN | ALA | ASN | THR | LYS | VAL | ALA | TYR |
|      |     | THR | ASP | ALA | ALA | THR | THR | ALA | THR | GLY | VAL | THR |
|      |     | LEU | THR | GLY | LEU | ARG | GLY | ALA | ALA | SER | PHE | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | ALA | ALA | GLU | LEU |
|      |     | ILE | ASP | GLY | GLY | PRO | GLY | GLY | ARG | ALA | GLU | LEU |
|      |     | LEU | LEU | LEU | LEU | THR | SER | PRO | SER | LEU | LEU | PHE |
|      |     | THR | THR | THR | THR | THR | THR | THR | ASN | THR | LEU | SER |
|      |     | ARG | GLU | GLU | GLU | GLU | THR | ARG | GLN | THR | ASP | ASN |
|      |     | LYS | ALA | ALA | ALA | ASN | GLN | THR | ALA | VAL | GLN | LEU |
|      |     | VAL | THR | GLN | THR | THR | GLN | THR | THR | THR | ASN | ASN |
|      |     | ALA | ASP | ASP | VAL | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
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|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
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|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
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|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
|      |     | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |
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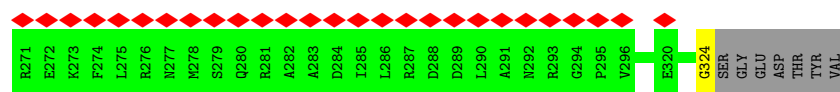
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | ALA | ALA | THR | THR | SER | THR | ALA | GLN | PRO | LYS | LEU | GLY | TRP | ASN | ARG | LEU | ARG | ALA | ASN | PRO | ARG | ILE | LEU | ILE | VAL | ALA | GLY | SER | ALA | ALA | VAL | ALA | ALA | ILE | VAL | VAL | VAL | MET | VAL | VAL | LEU | TRP | TYR | ARG | THR | LEU | PHE | SER | ASN | LEU | SER | ASP | PRO | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

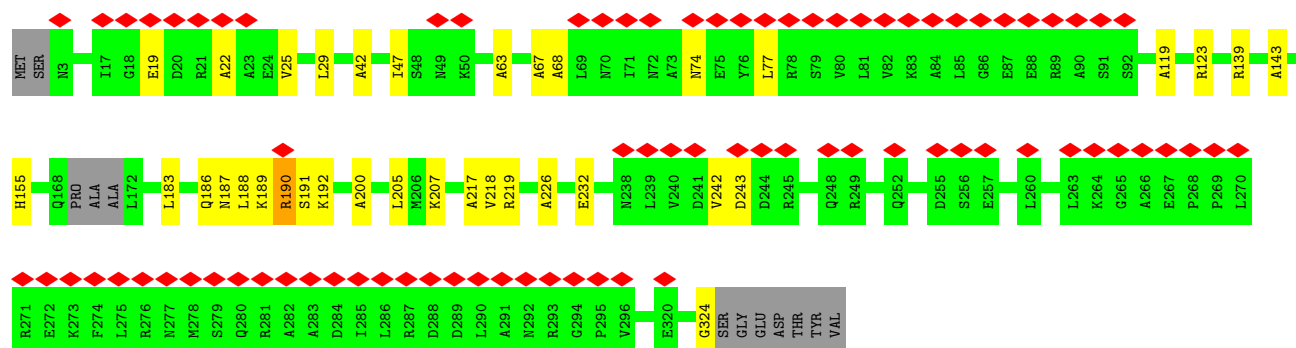
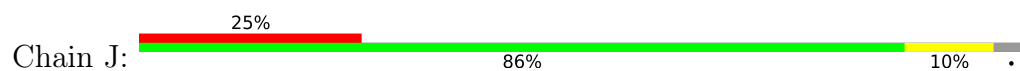


• Molecule 2: Flagellar motor switch protein FliG

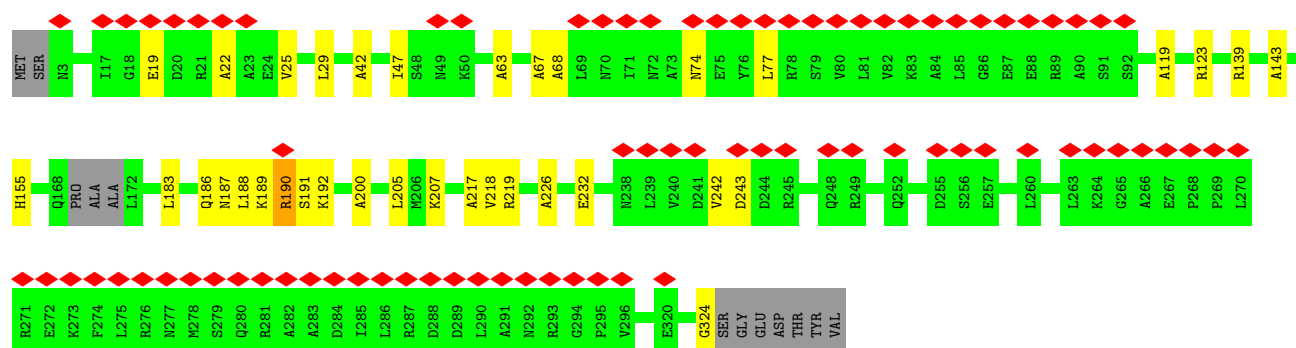
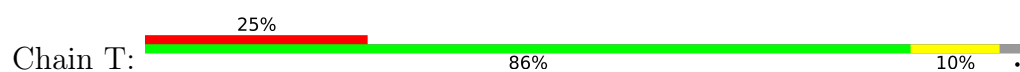




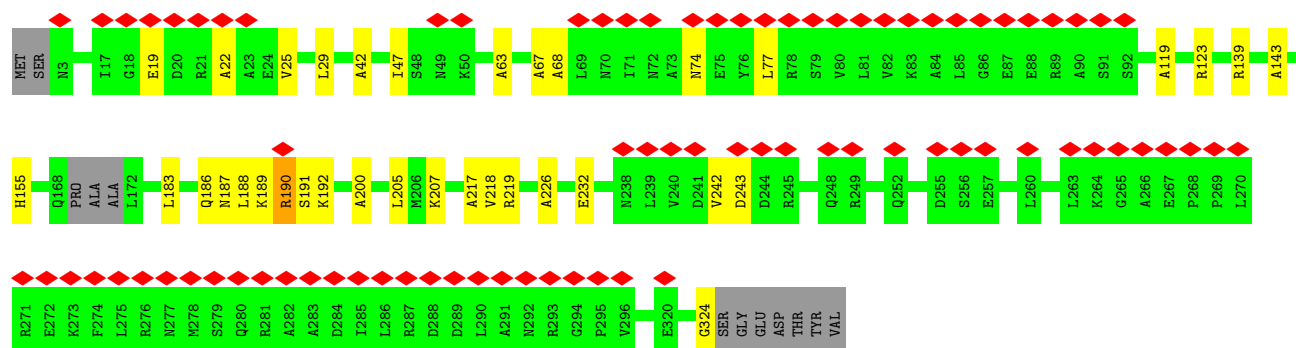
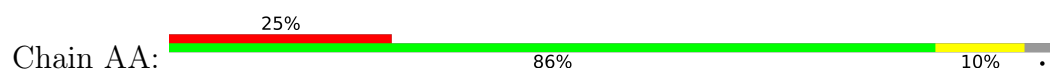
• Molecule 2: Flagellar motor switch protein FliG



• Molecule 2: Flagellar motor switch protein FliG

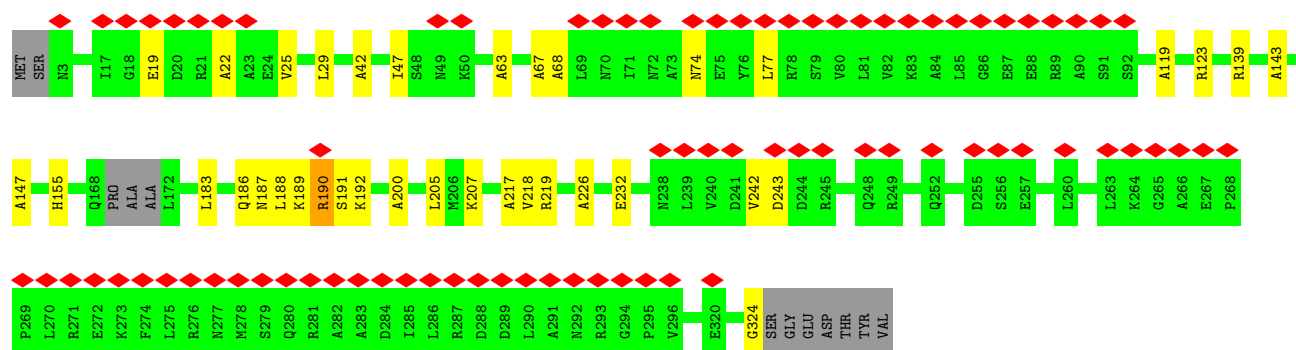


• Molecule 2: Flagellar motor switch protein FliG



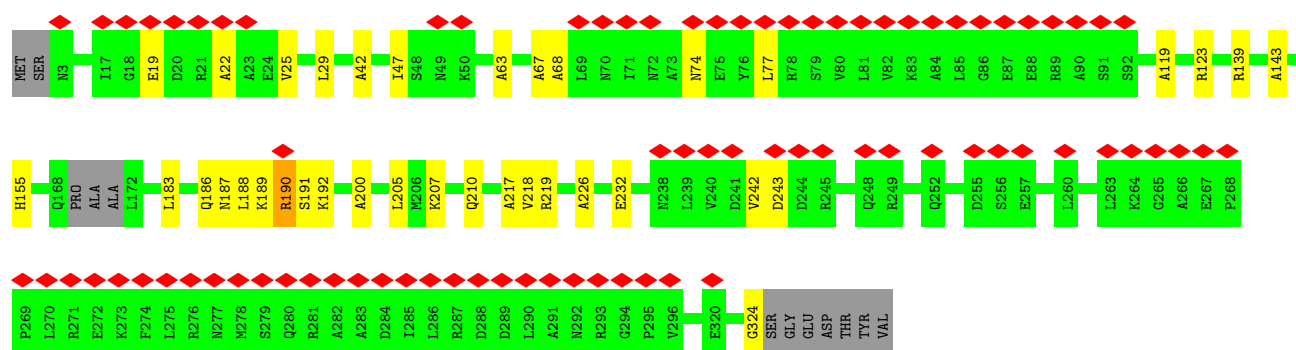
• Molecule 2: Flagellar motor switch protein FliG

Chain GA: 



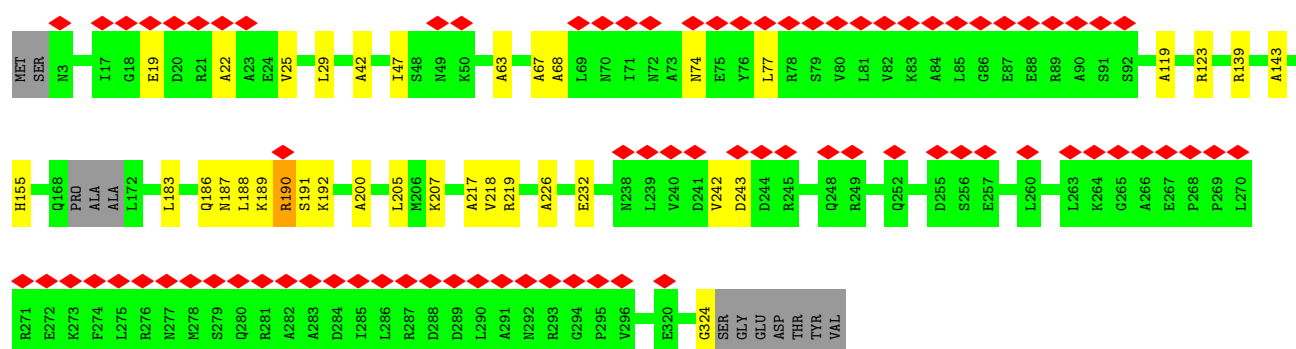
• Molecule 2: Flagellar motor switch protein FlgG

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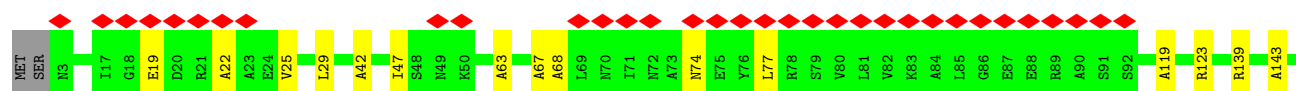
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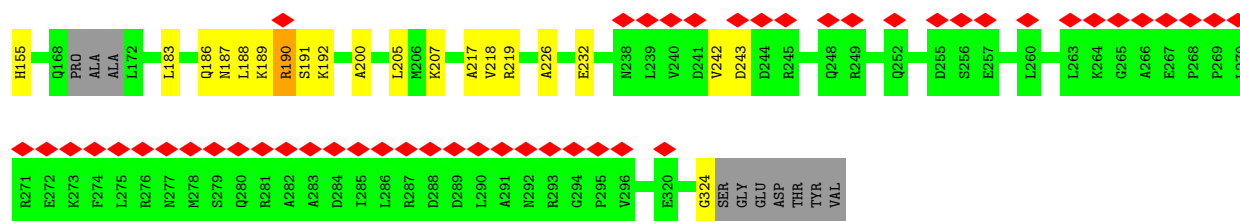
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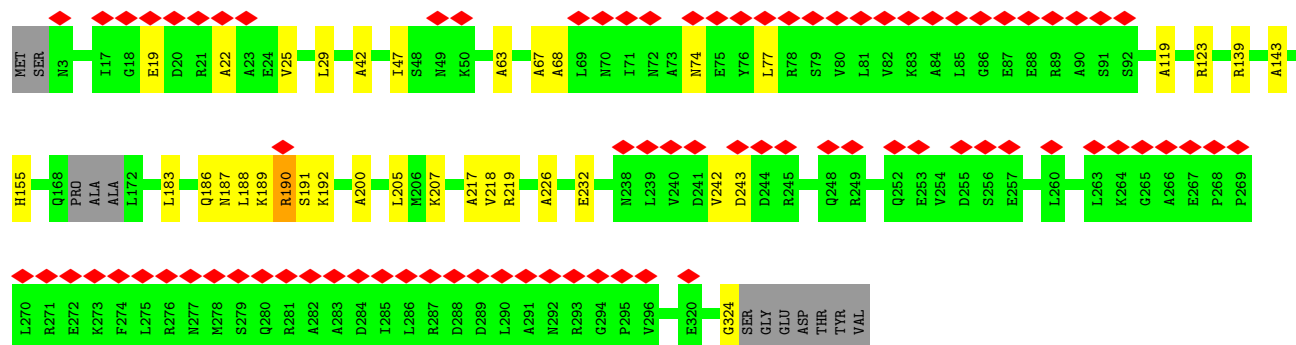
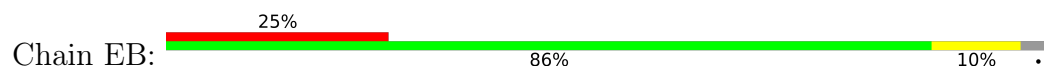
• Molecule 2: Flagellar motor switch protein FlgG

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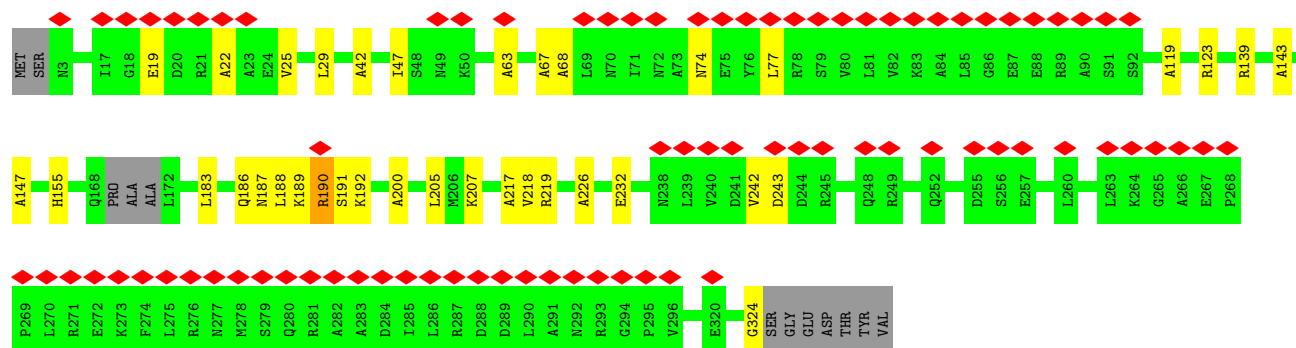
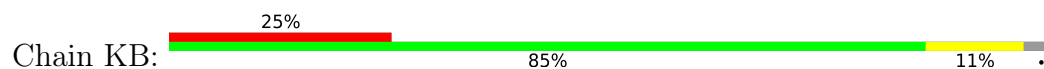




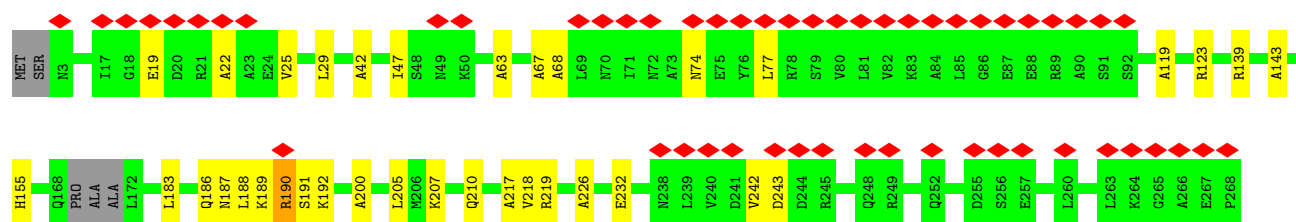
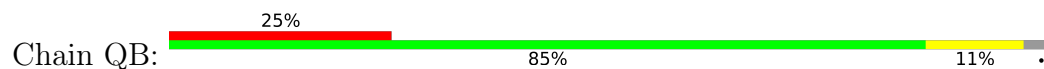
• Molecule 2: Flagellar motor switch protein FlhG

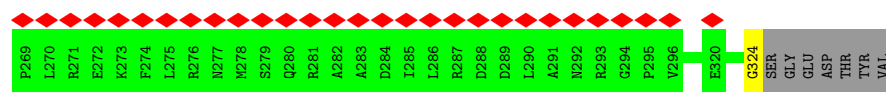


• Molecule 2: Flagellar motor switch protein FlhG



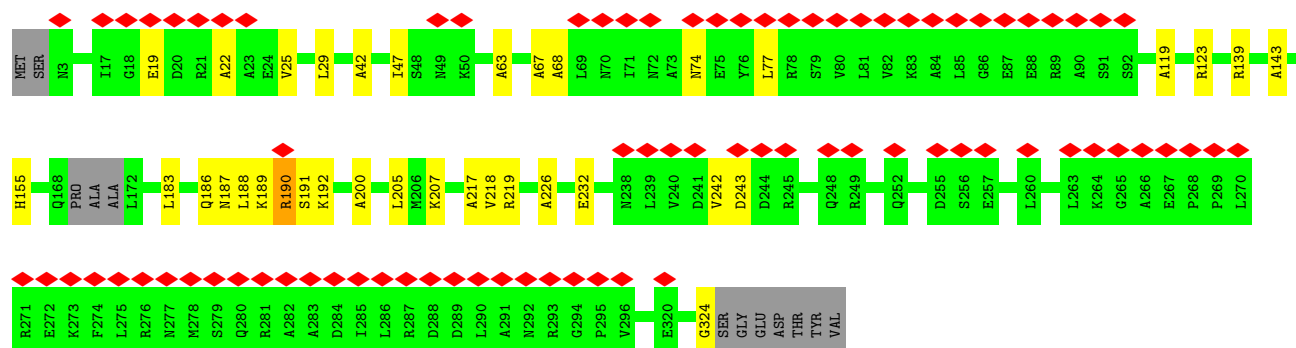
• Molecule 2: Flagellar motor switch protein FlhG





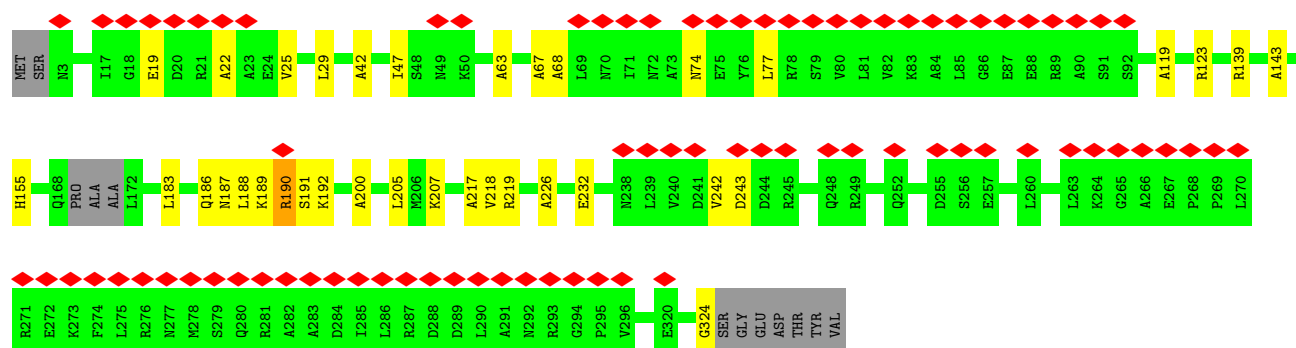
• Molecule 2: Flagellar motor switch protein FliG

Chain WB: 25% 86% 10% .



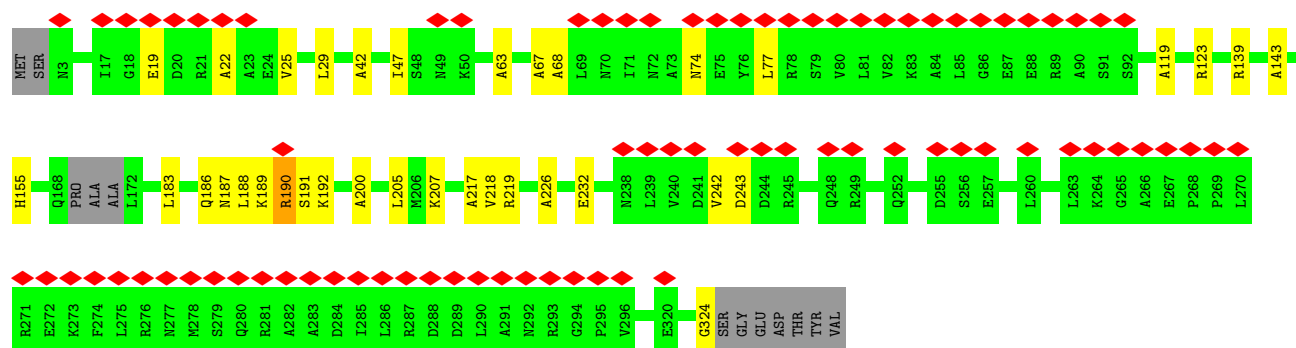
• Molecule 2: Flagellar motor switch protein FliG

Chain CC: 25% 86% 10% .



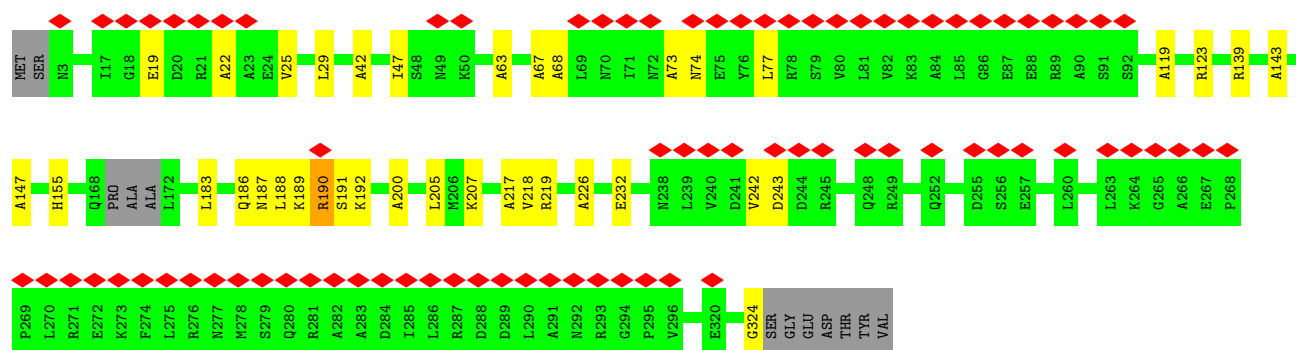
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Chain IC: 25% 86% 10% .



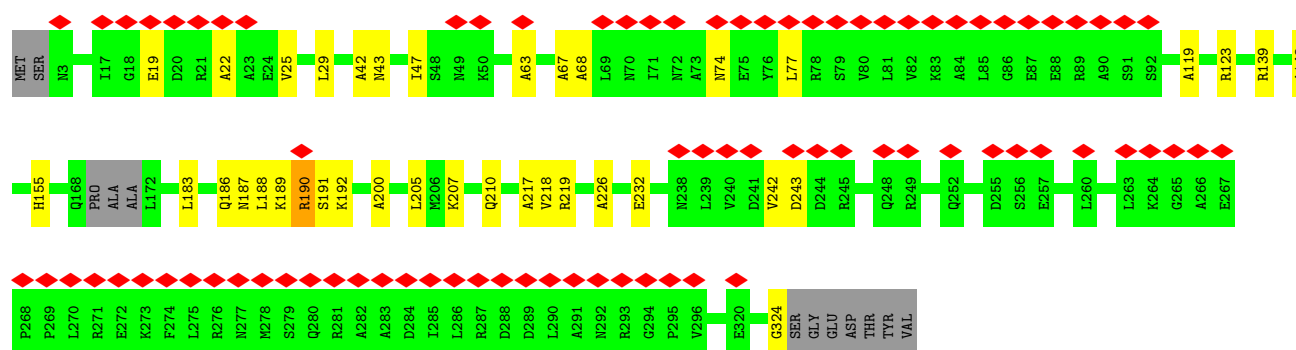
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Chain OC: 



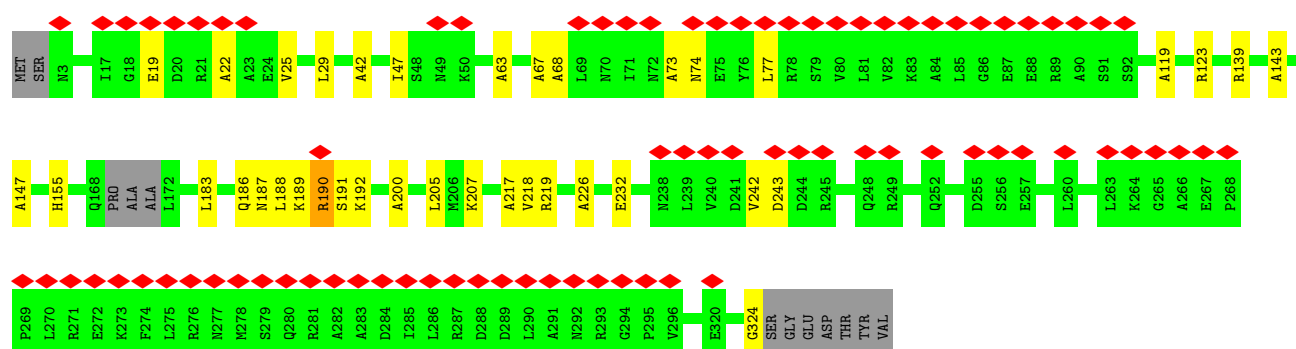
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Chain UC: 



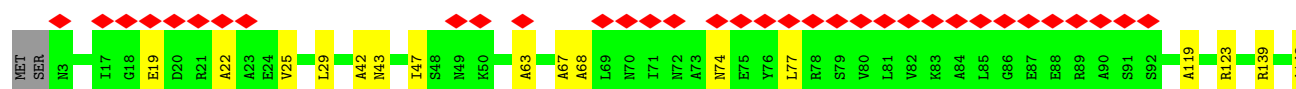
• Molecule 2: Flagellar motor switch protein FliG

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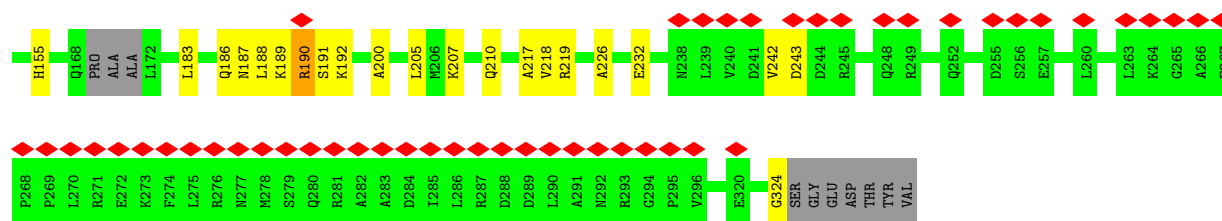


• Molecule 2: Flagellar motor switch protein FliG

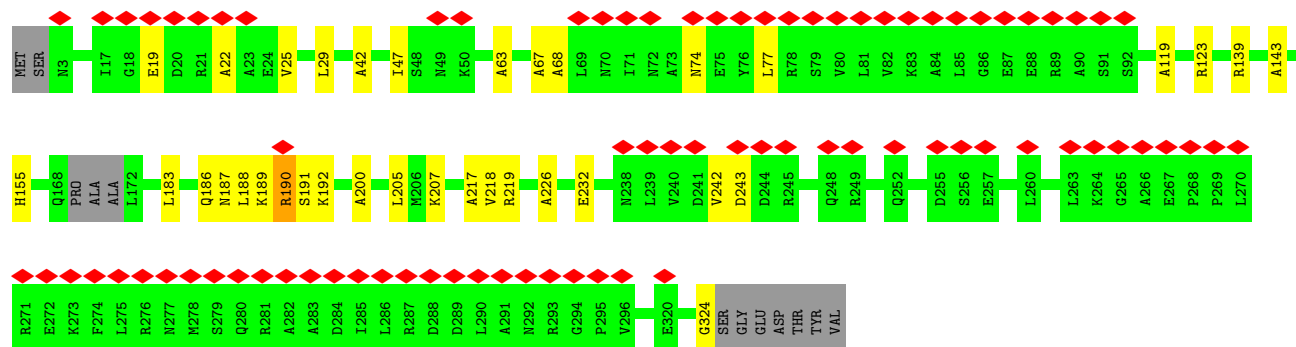
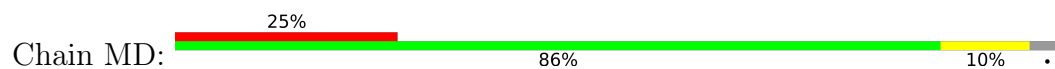
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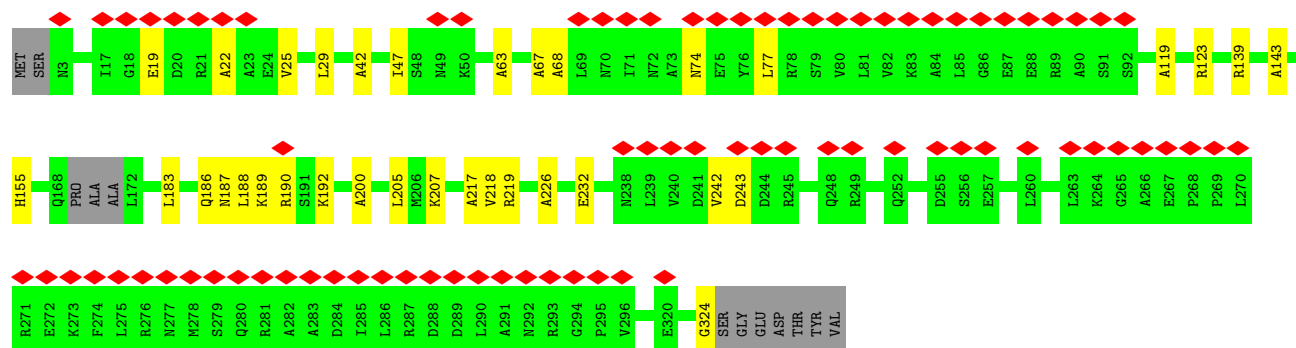
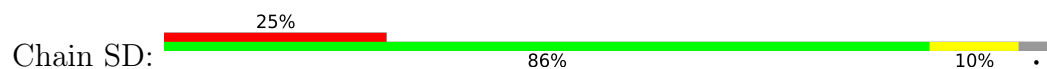




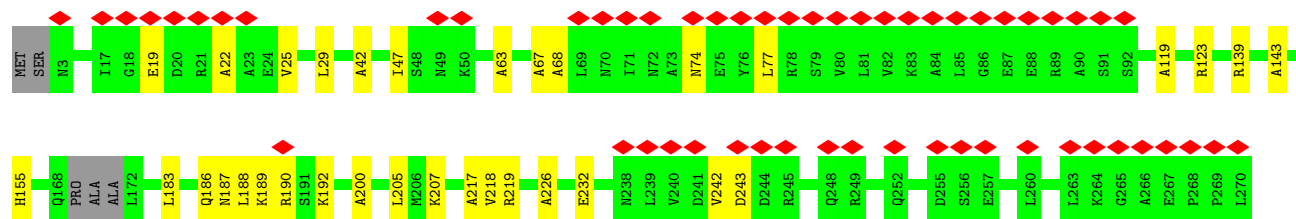
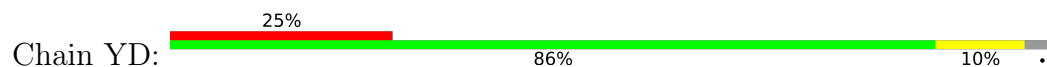
• Molecule 2: Flagellar motor switch protein FlhG

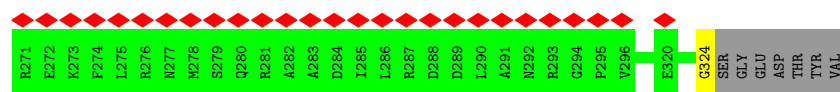


• Molecule 2: Flagellar motor switch protein FlhG



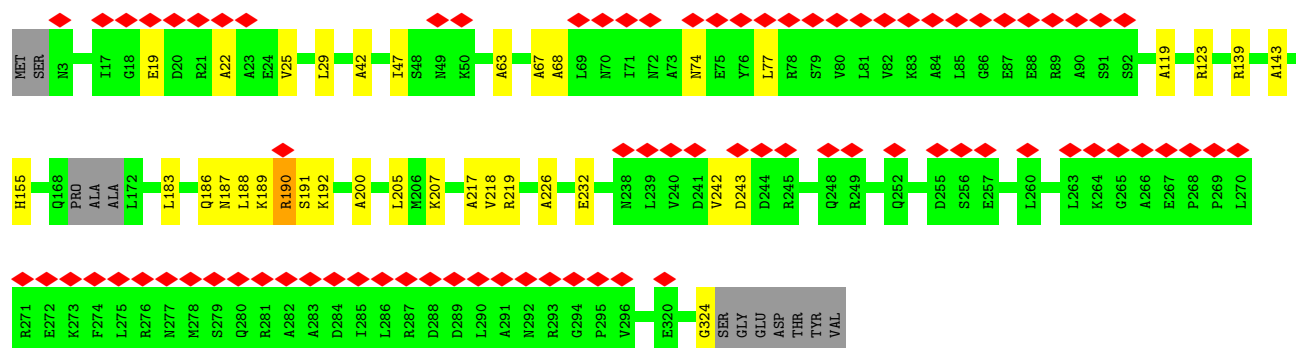
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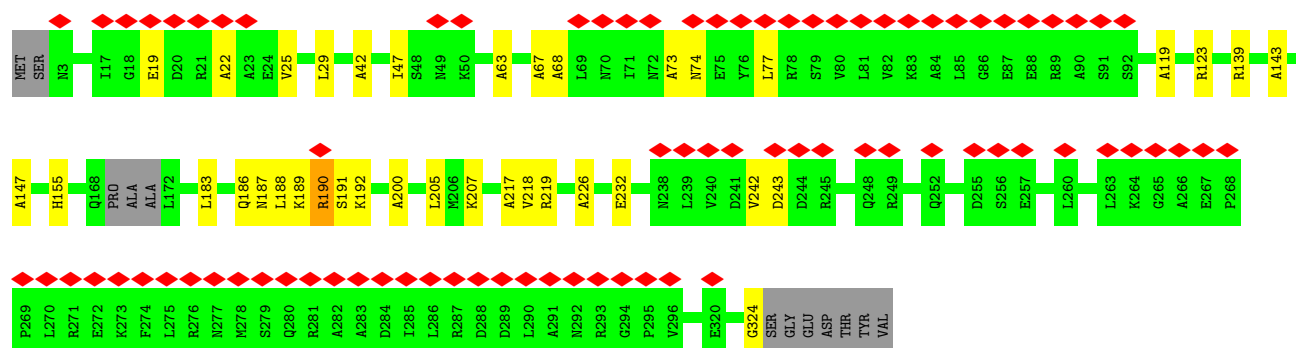
• Molecule 2: Flagellar motor switch protein FltG

Chain EE: 25% 86% 10% .



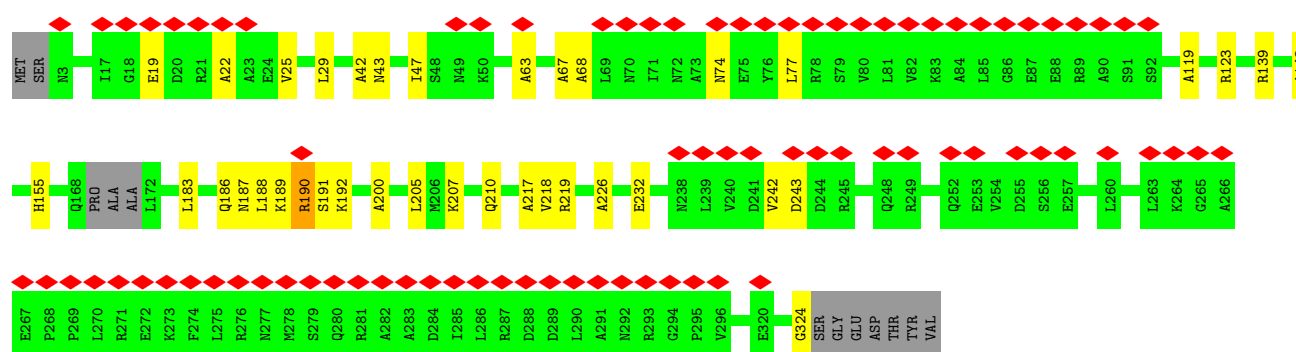
• Molecule 2: Flagellar motor switch protein FltG

Chain KE: 25% 85% 11% .

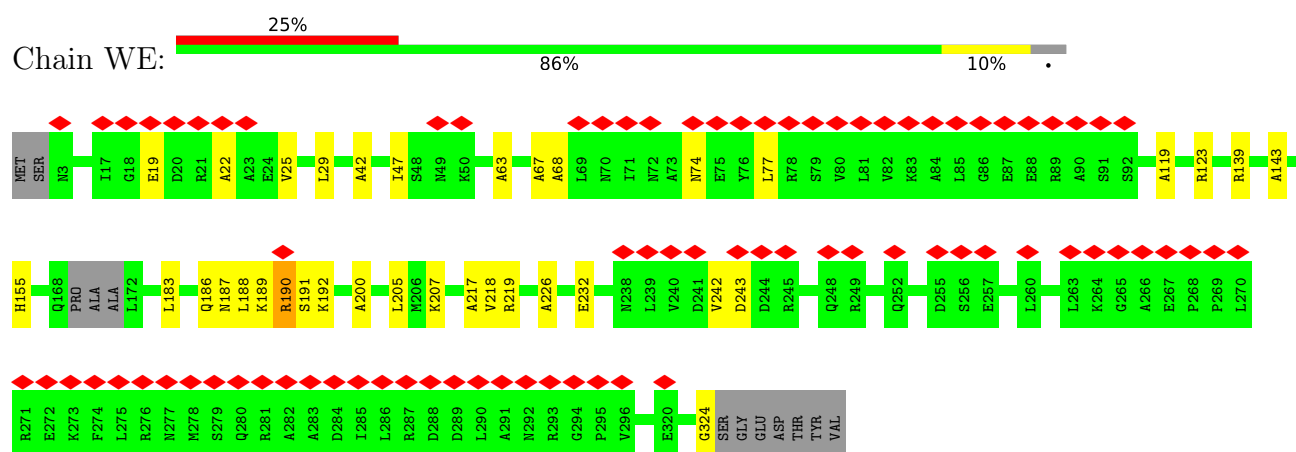


• Molecule 2: Flagellar motor switch protein FltG

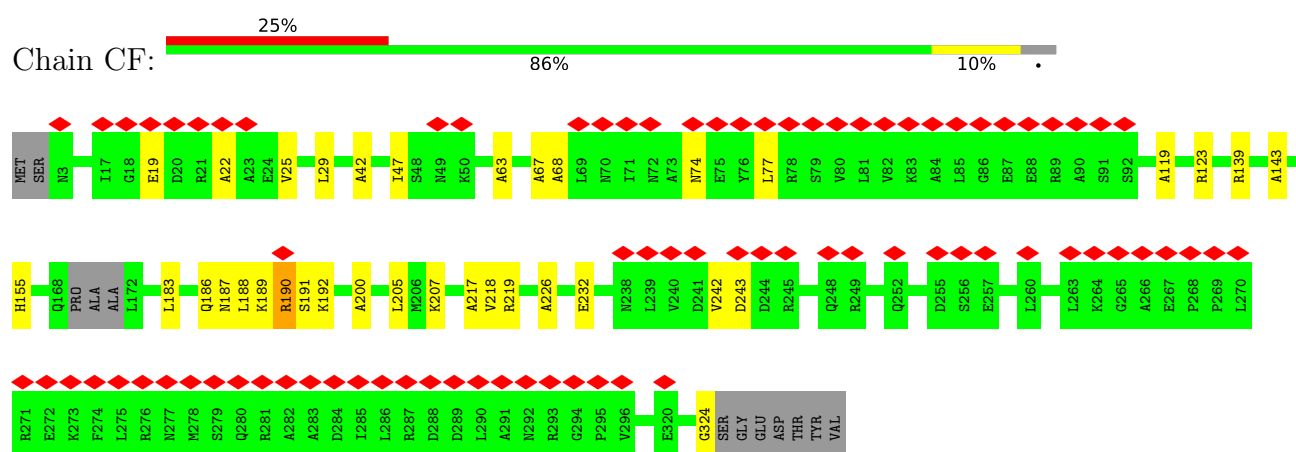
Chain QE: 26% 85% 11% .



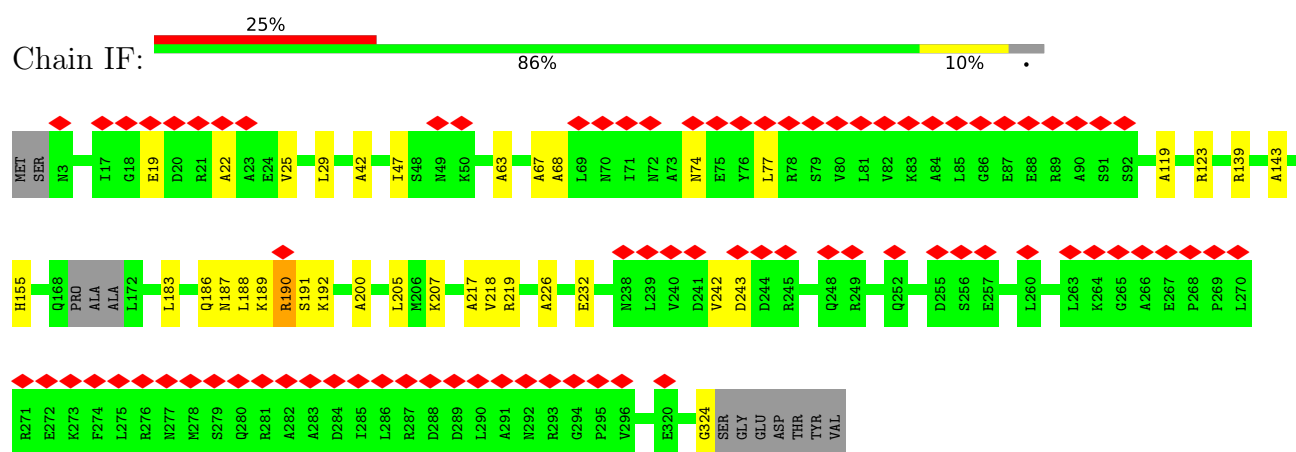
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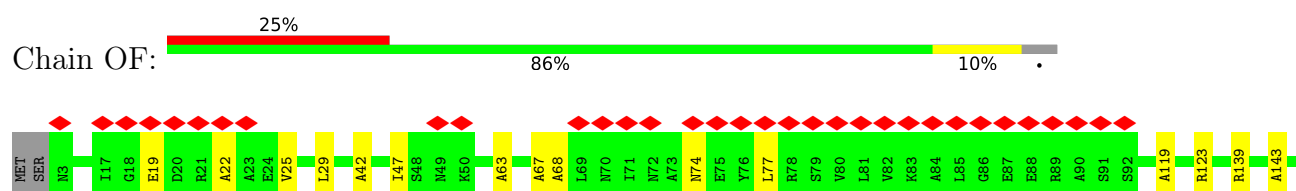
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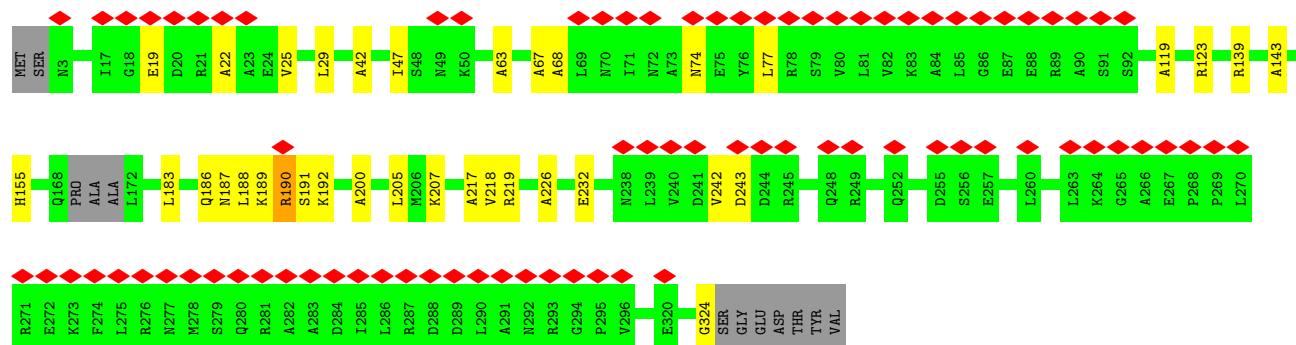
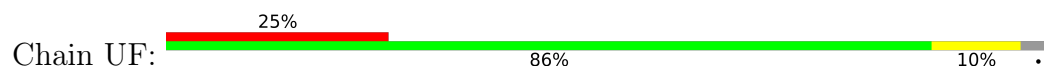
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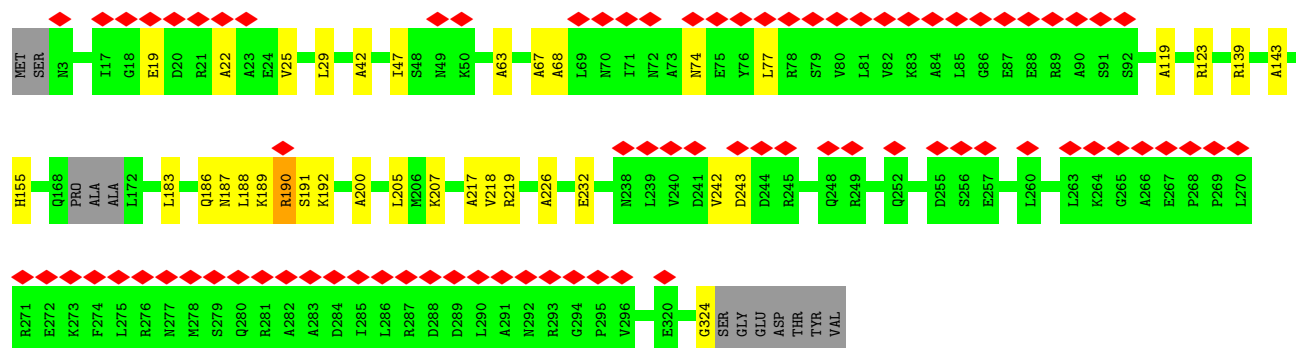
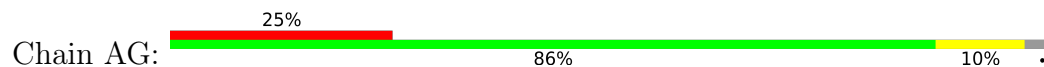
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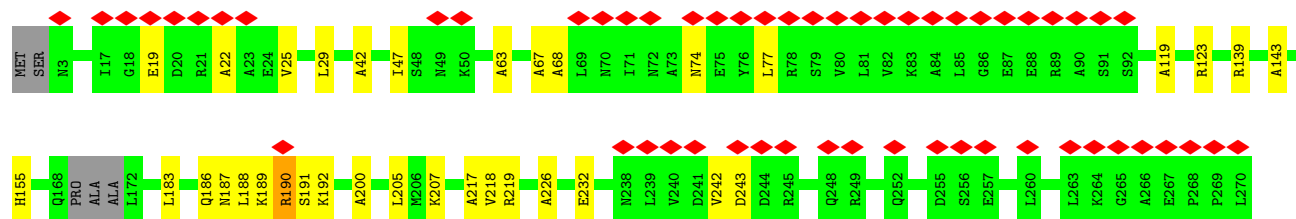
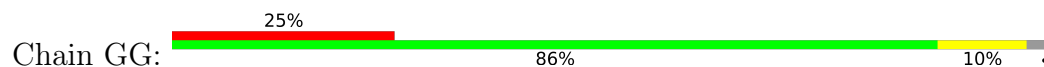
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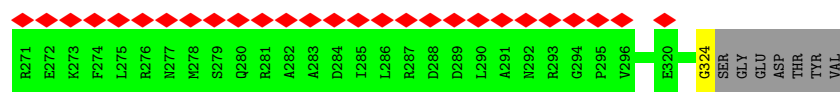


- Molecule 2: Flagellar motor switch protein FliG

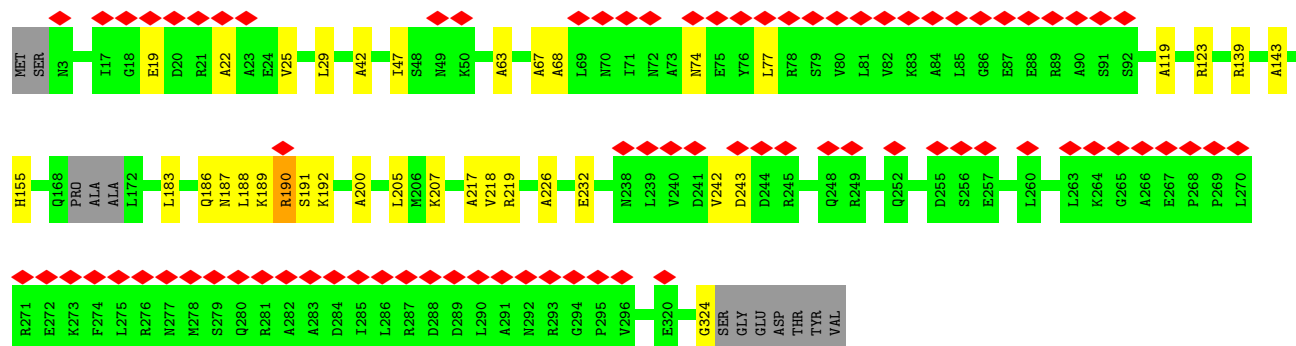
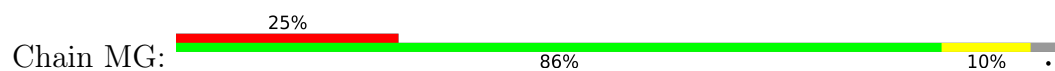


- Molecule 2: Flagellar motor switch protein FliG

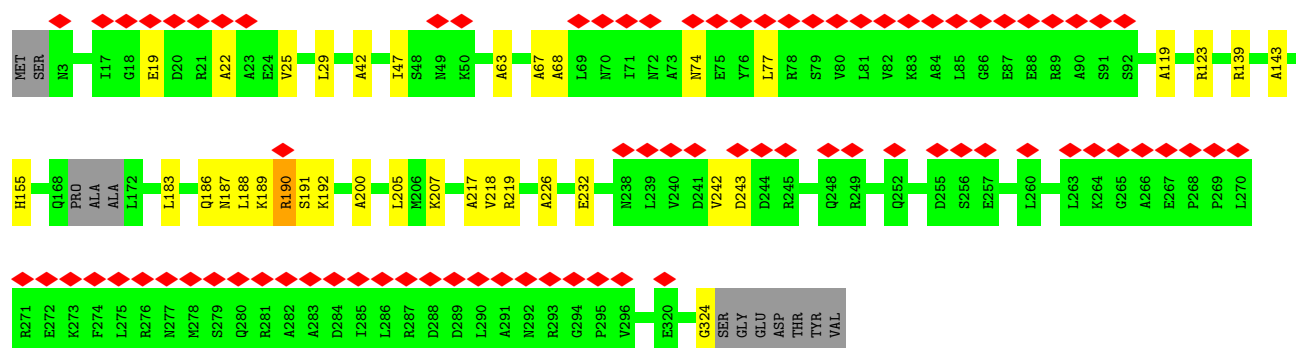
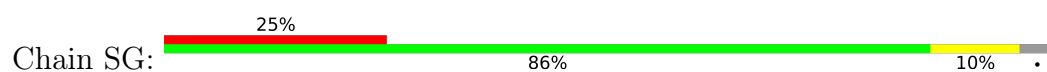




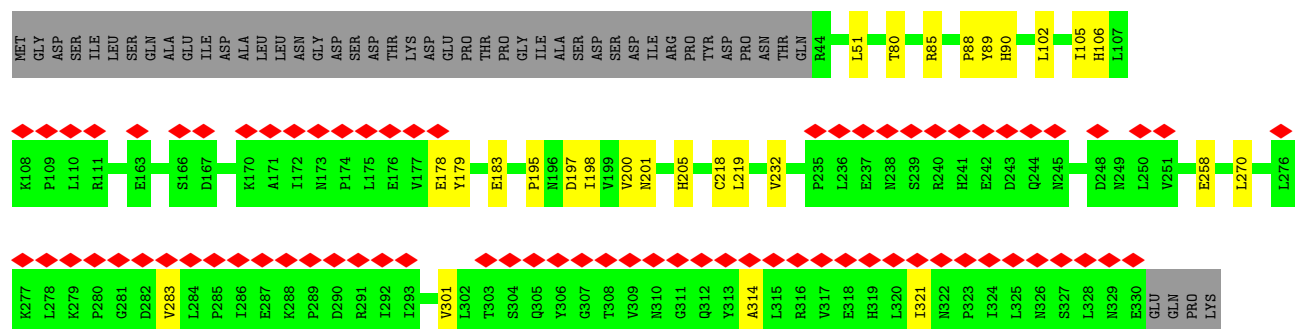
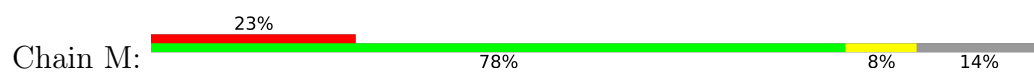
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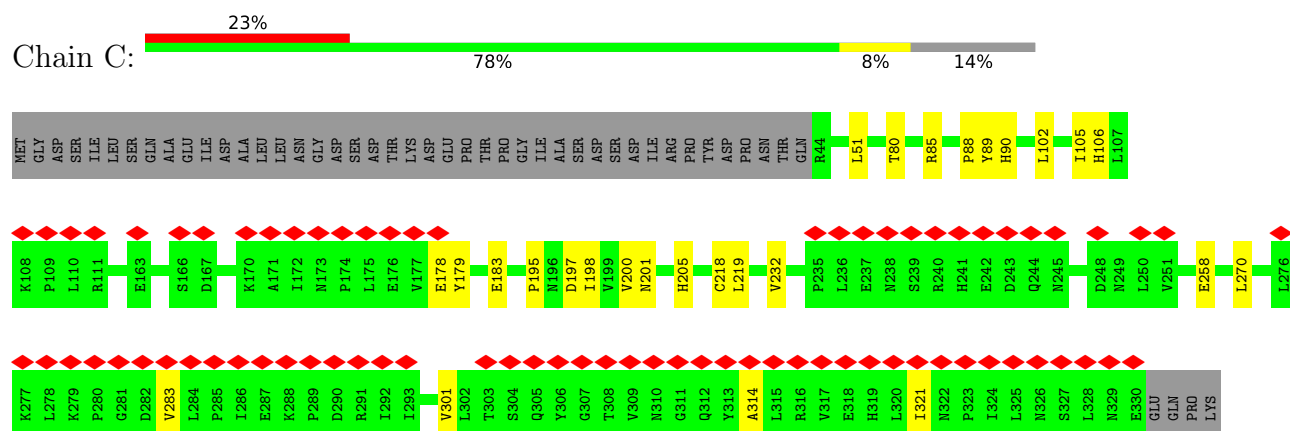
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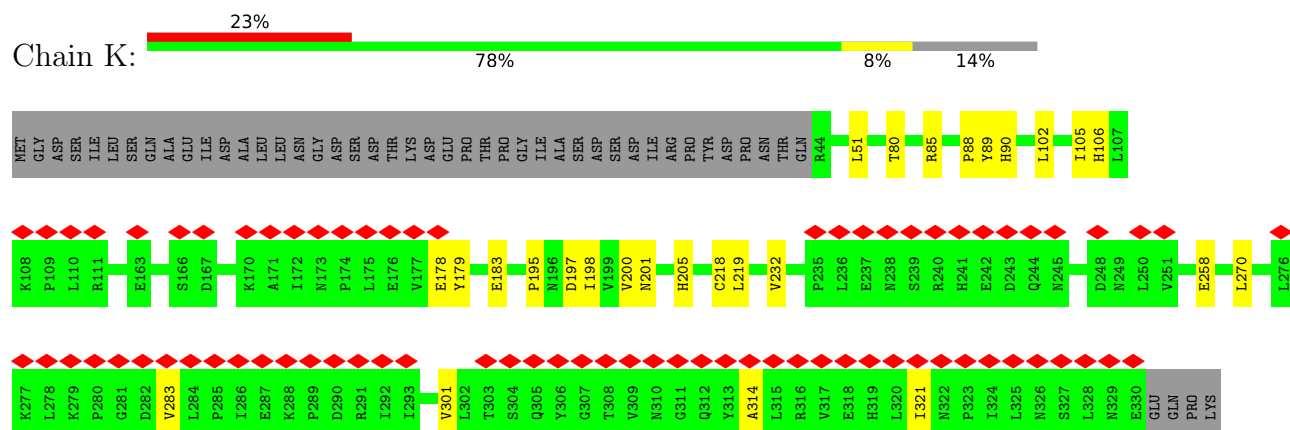
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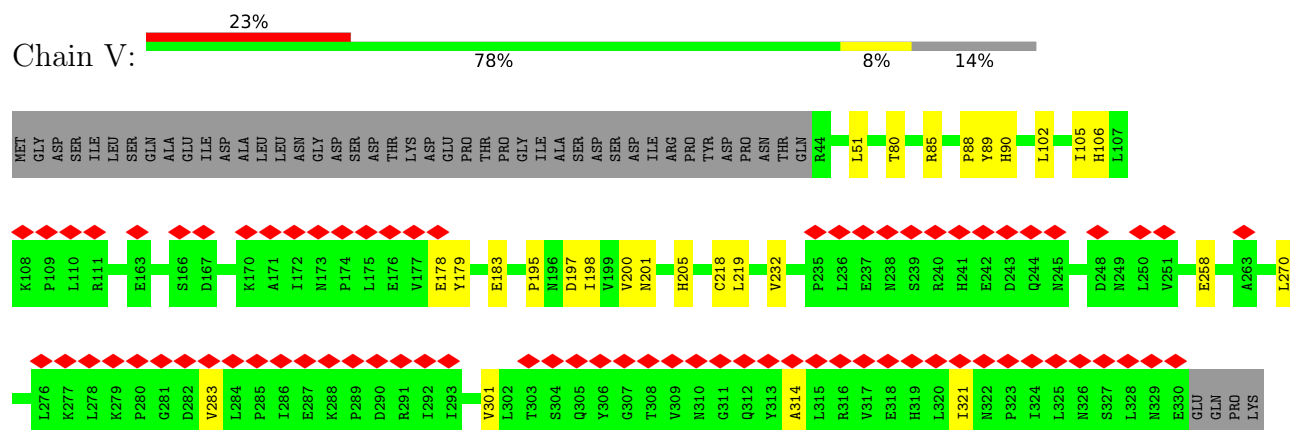
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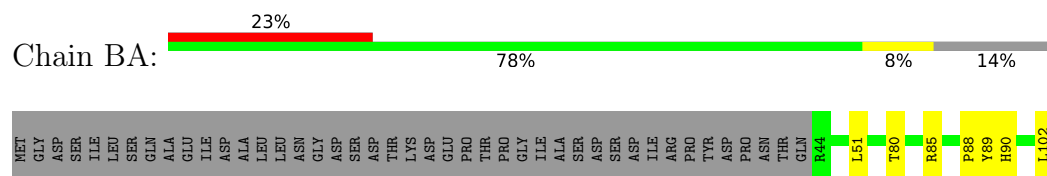
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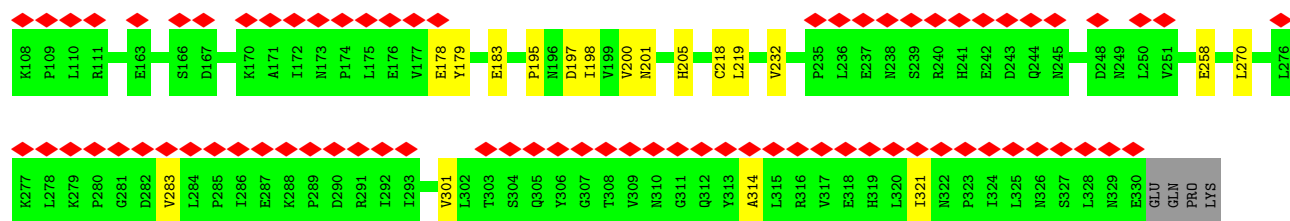


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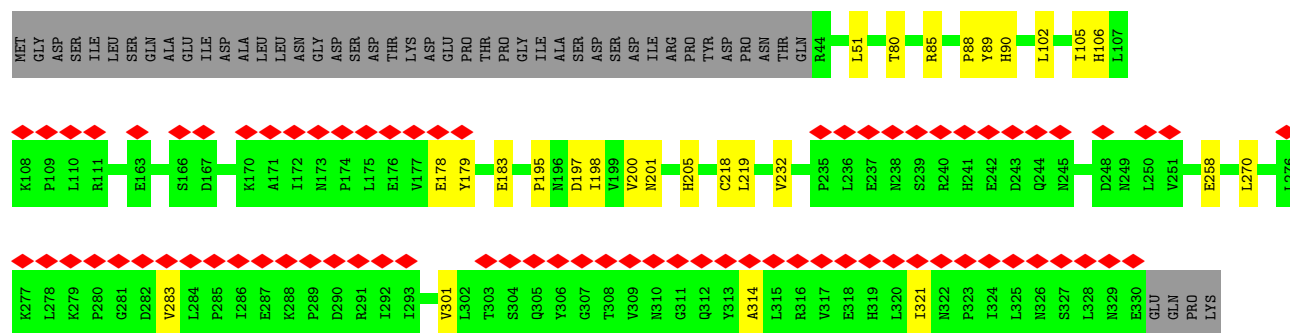
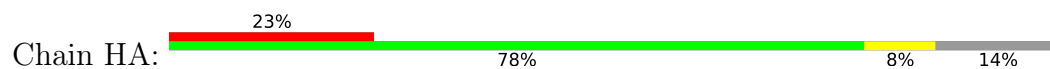


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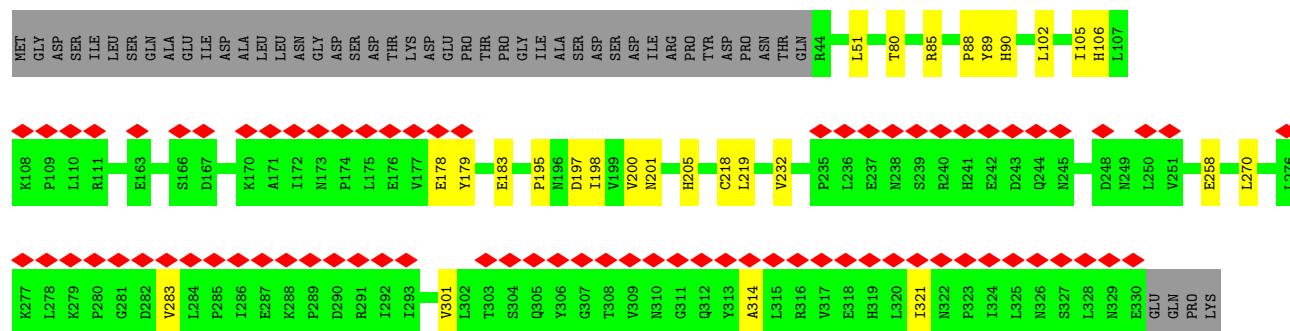
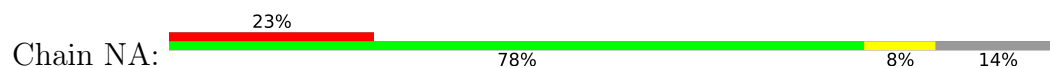




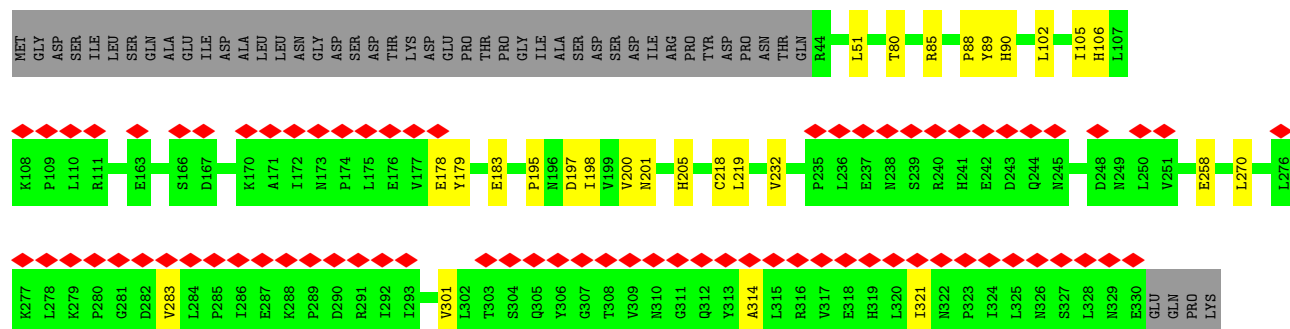
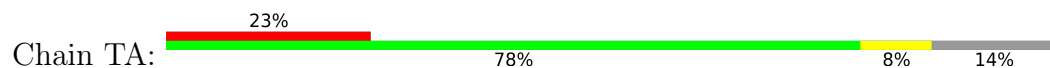
• Molecule 3: Flagellar motor switch protein FlIM



• Molecule 3: Flagellar motor switch protein FlIM

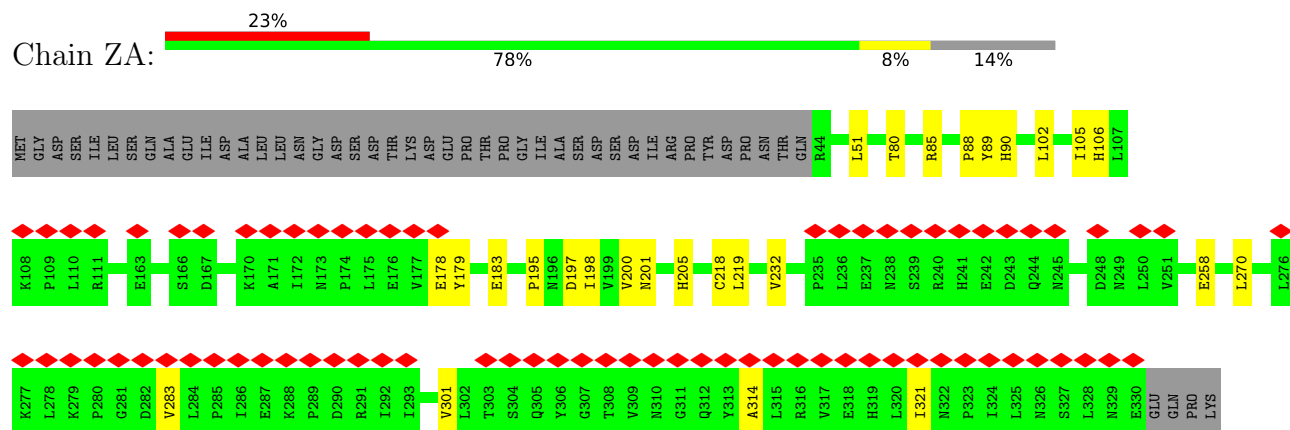


• Molecule 3: Flagellar motor switch protein FlIM



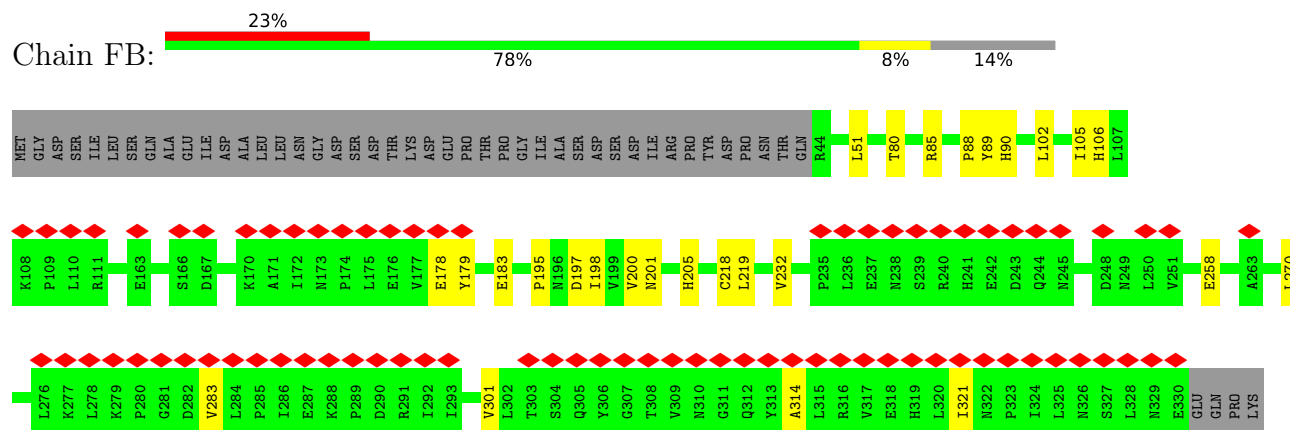
- Molecule 3: Flagellar motor switch protein FlIM

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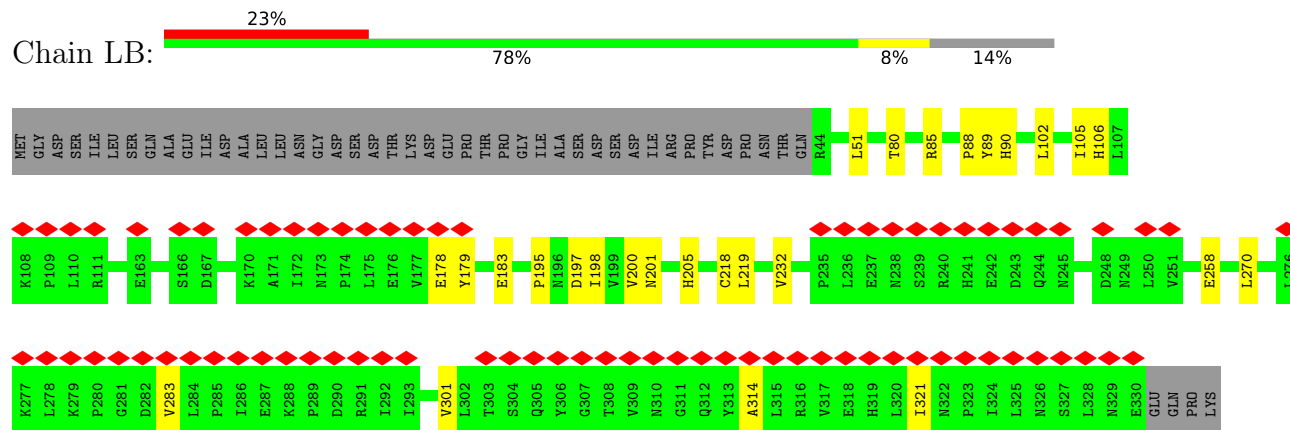
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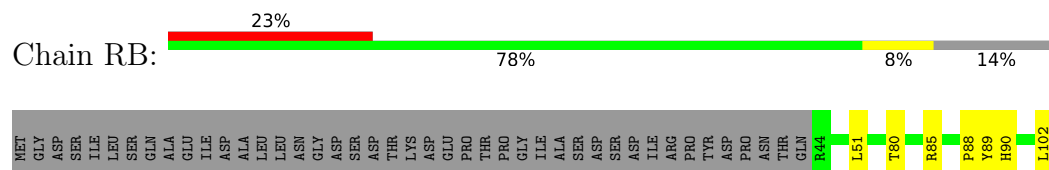
- Molecule 3: Flagellar motor switch protein FlIM

Chain LB:

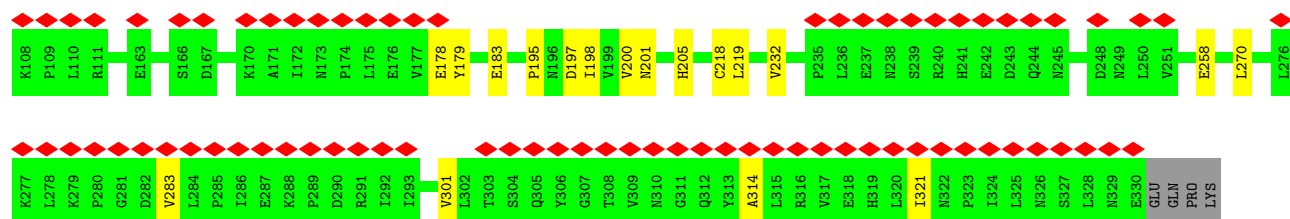


- Molecule 3: Flagellar motor switch protein FlIM

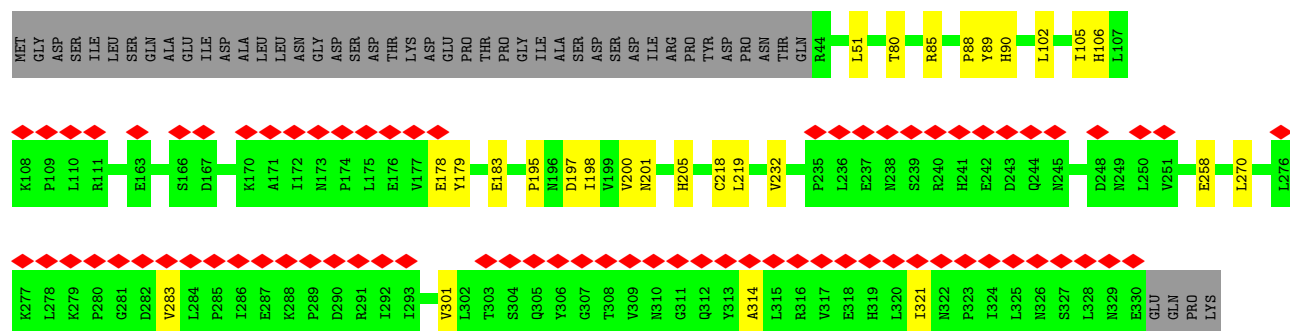
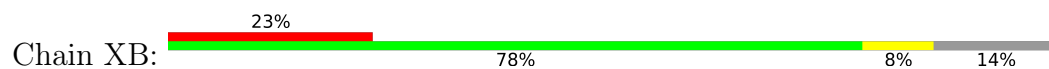
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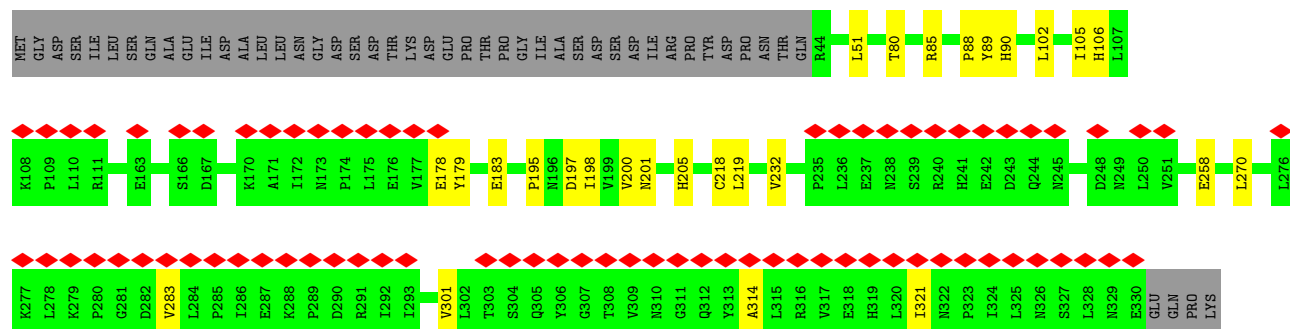
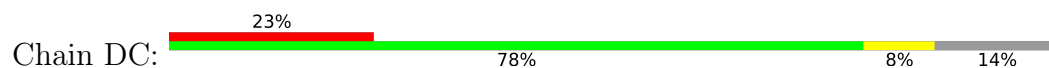




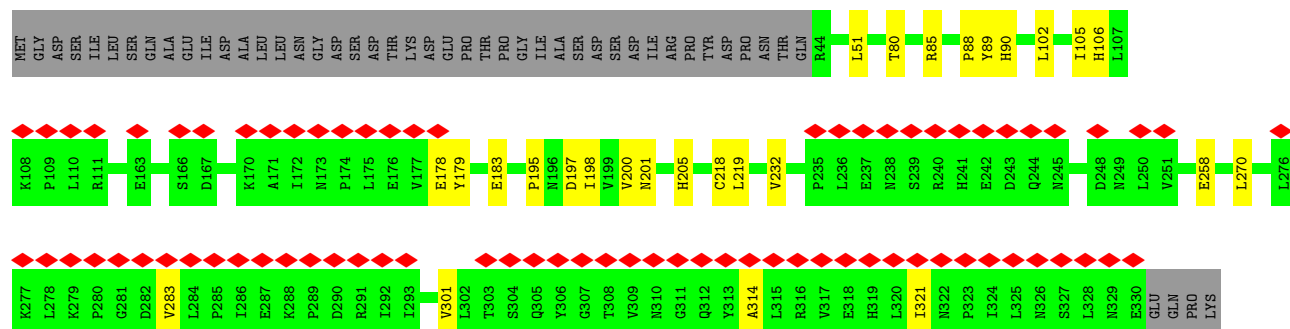
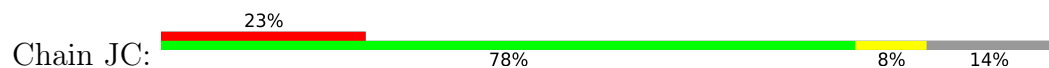
• Molecule 3: Flagellar motor switch protein FliM



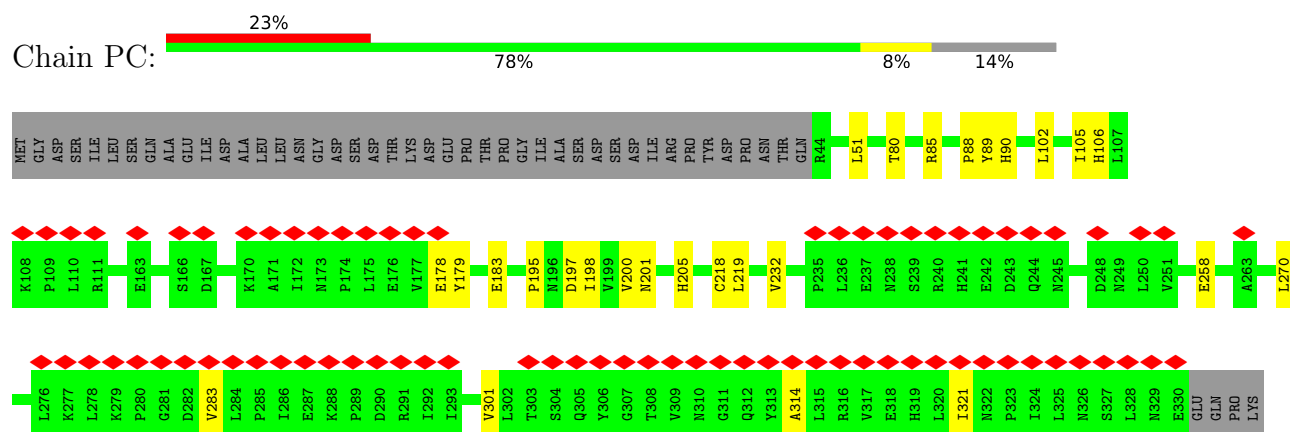
• Molecule 3: Flagellar motor switch protein FliM



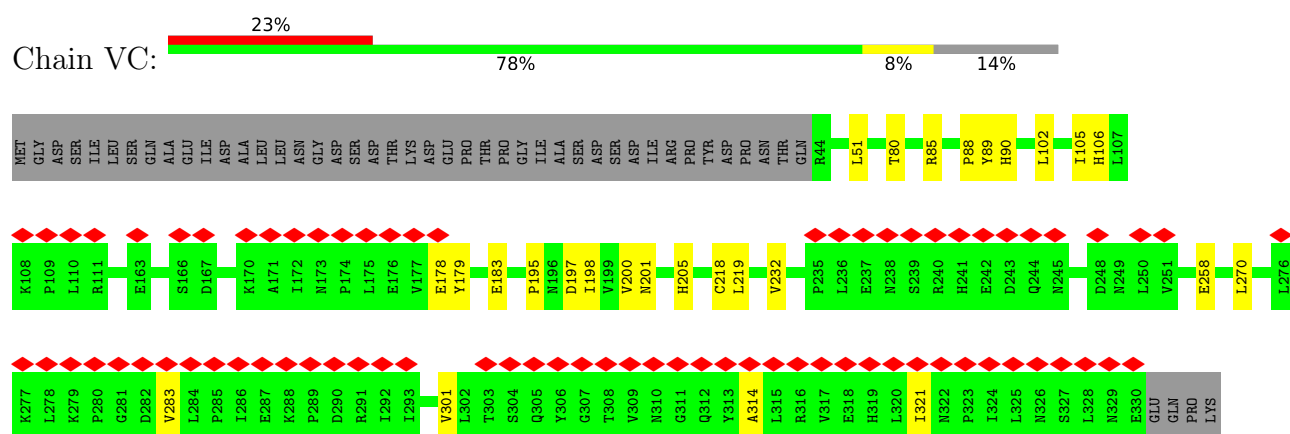
• Molecule 3: Flagellar motor switch protein FliM



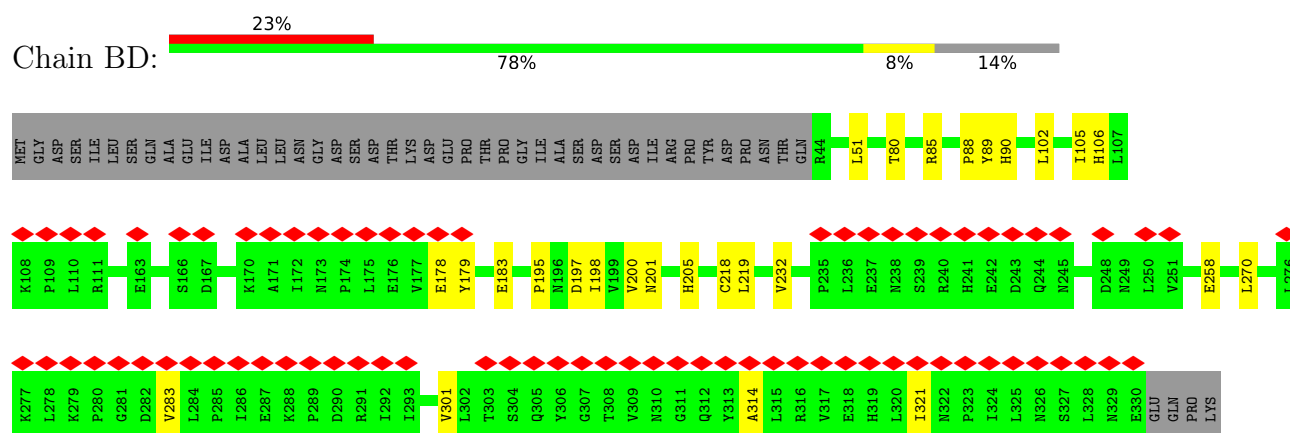
## ● Molecule 3: Flagellar motor switch protein FlIM



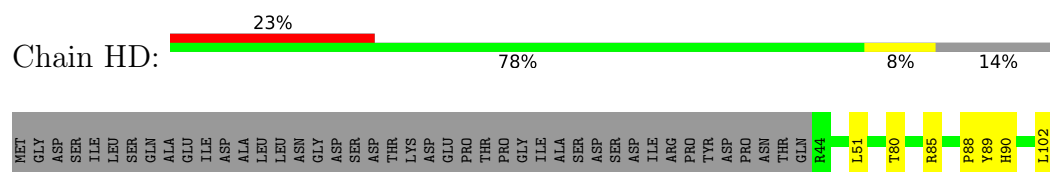
## ● Molecule 3: Flagellar motor switch protein FlIM

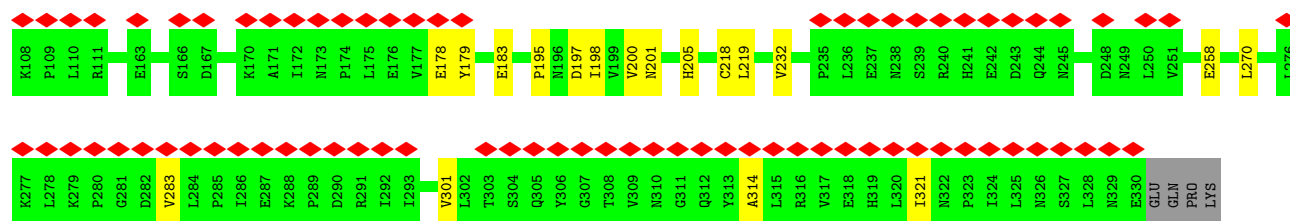


## ● Molecule 3: Flagellar motor switch protein FlIM

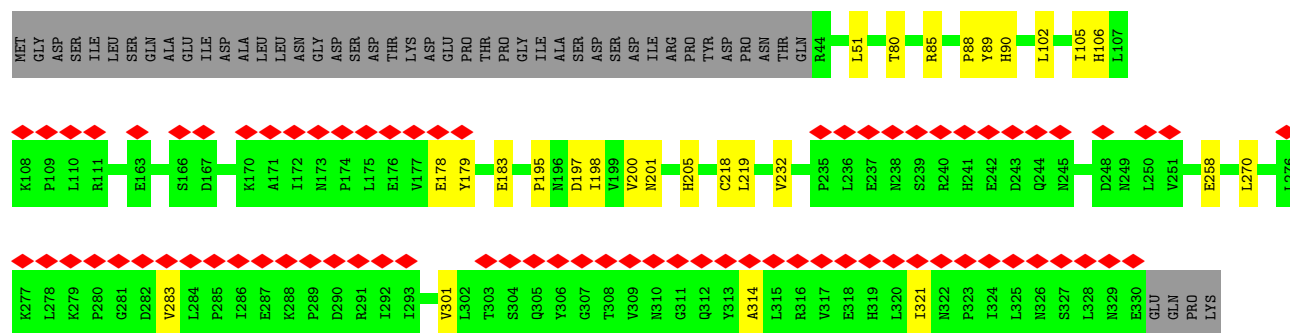
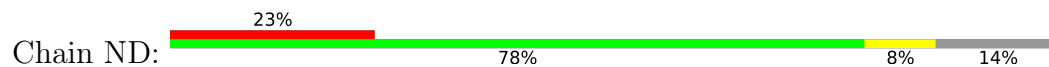


## ● Molecule 3: Flagellar motor switch protein FlIM

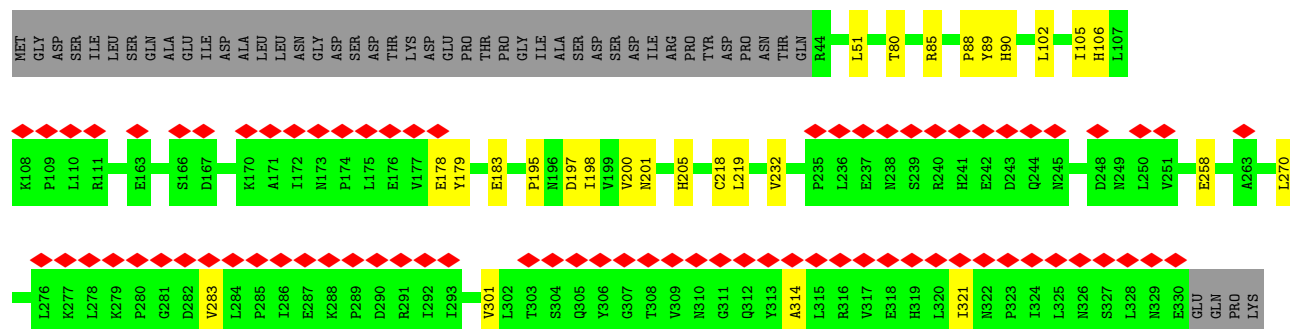
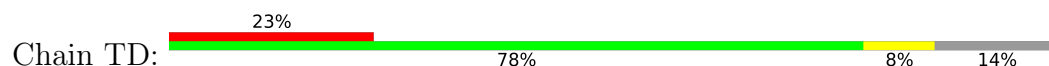




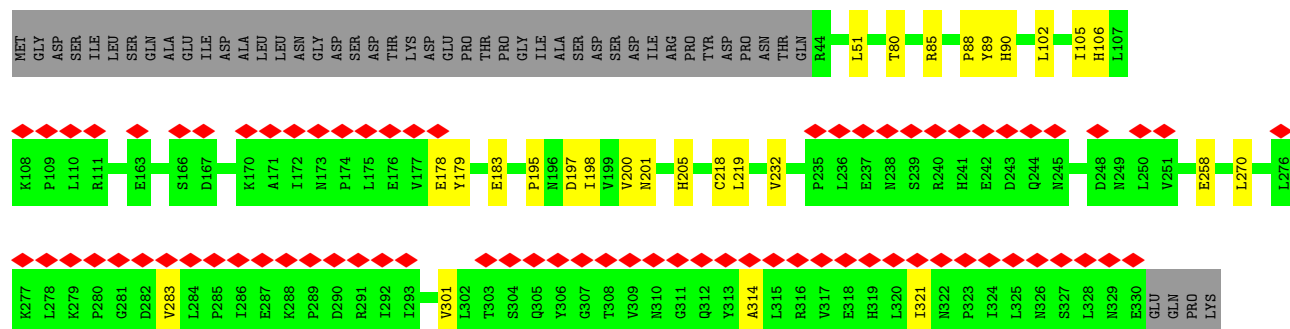
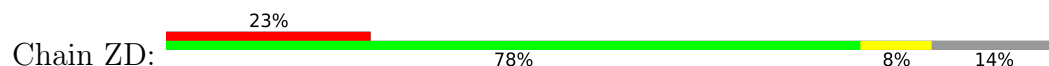
• Molecule 3: Flagellar motor switch protein FliM



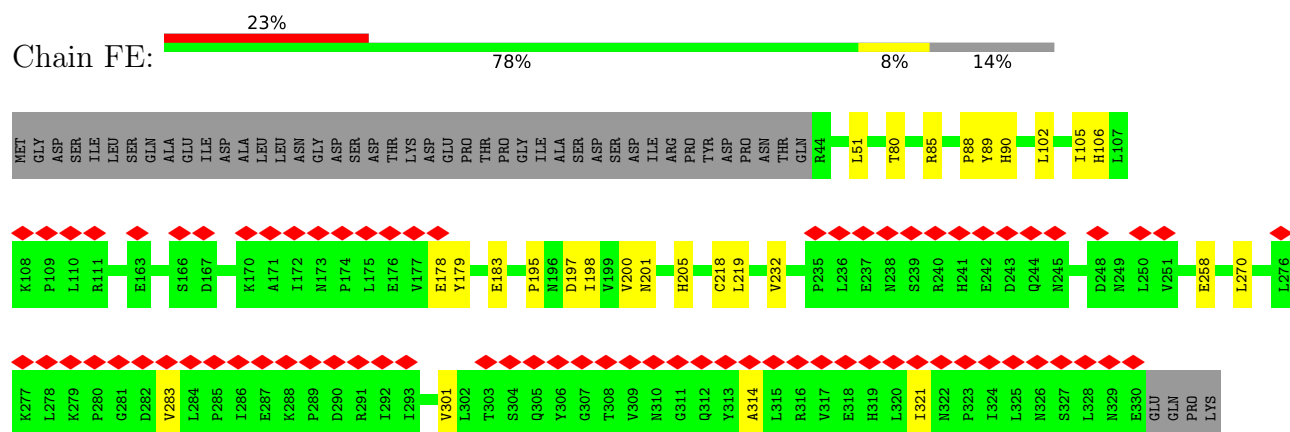
• Molecule 3: Flagellar motor switch protein FliM



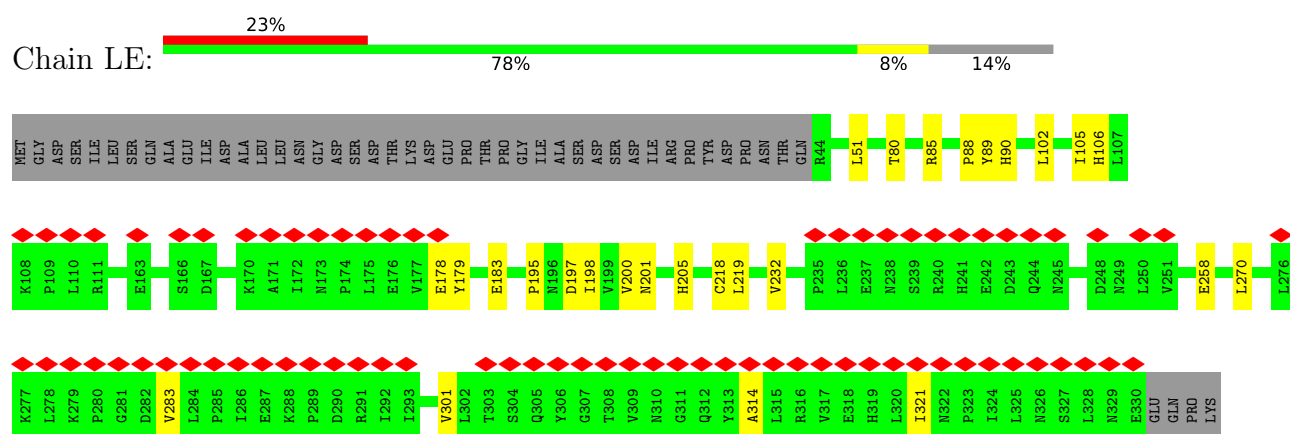
• Molecule 3: Flagellar motor switch protein FliM



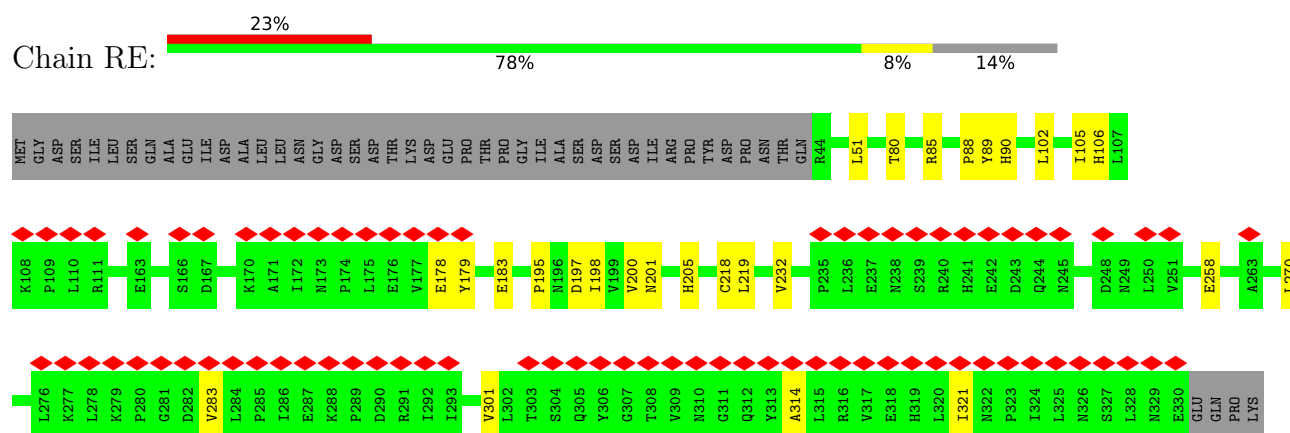
## ● Molecule 3: Flagellar motor switch protein FlIM



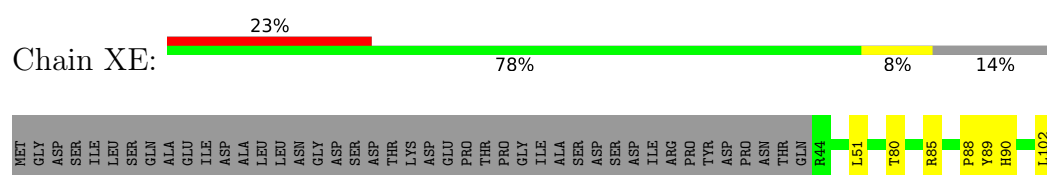
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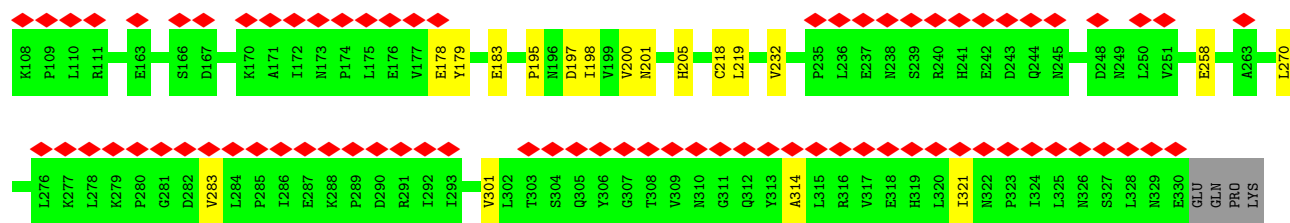


## ● Molecule 3: Flagellar motor switch protein FlIM

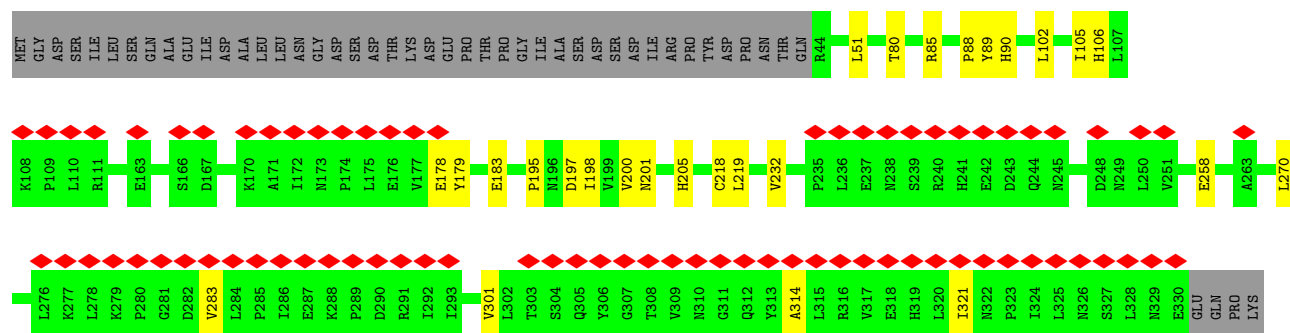
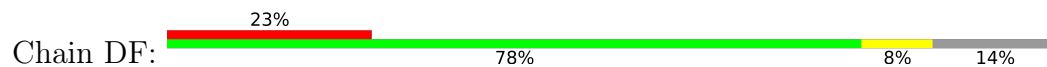


## ● Molecule 3: Flagellar motor switch protein FlIM

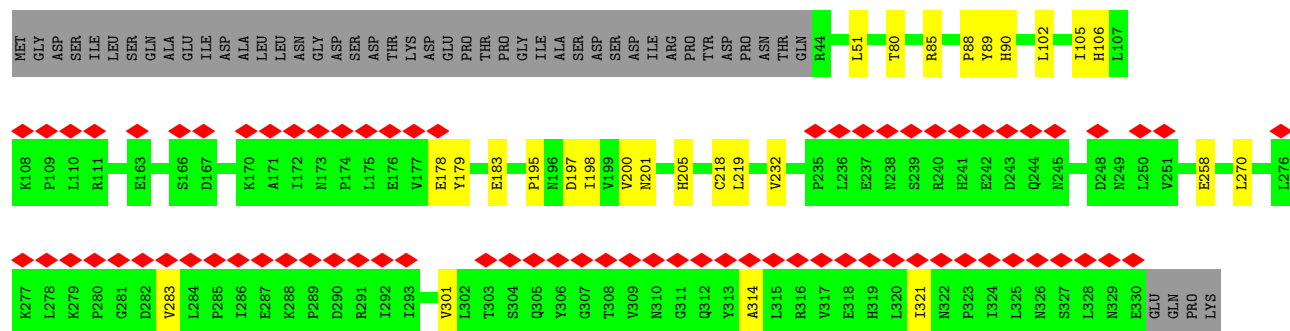
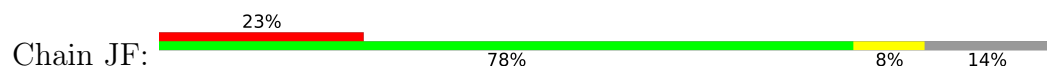




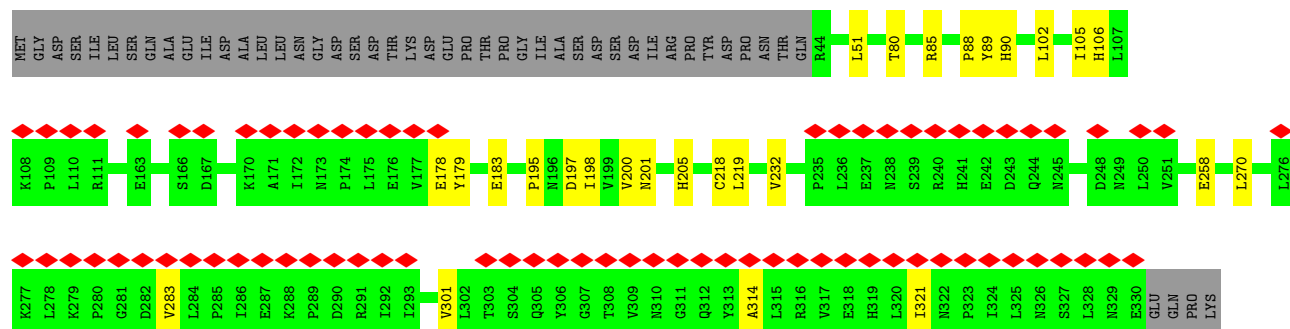
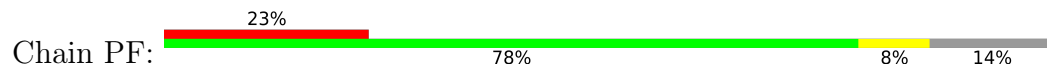
• Molecule 3: Flagellar motor switch protein FliM



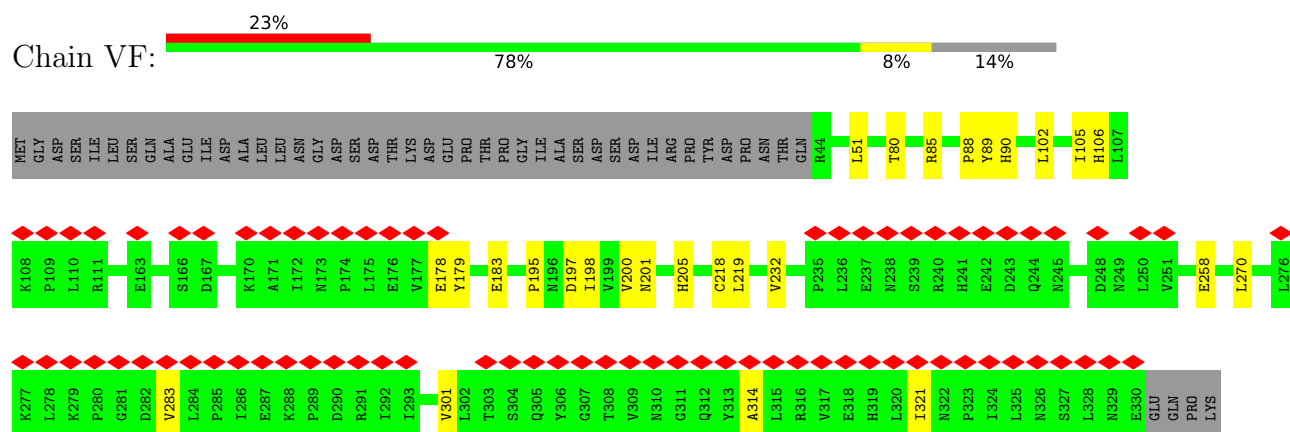
• Molecule 3: Flagellar motor switch protein FliM



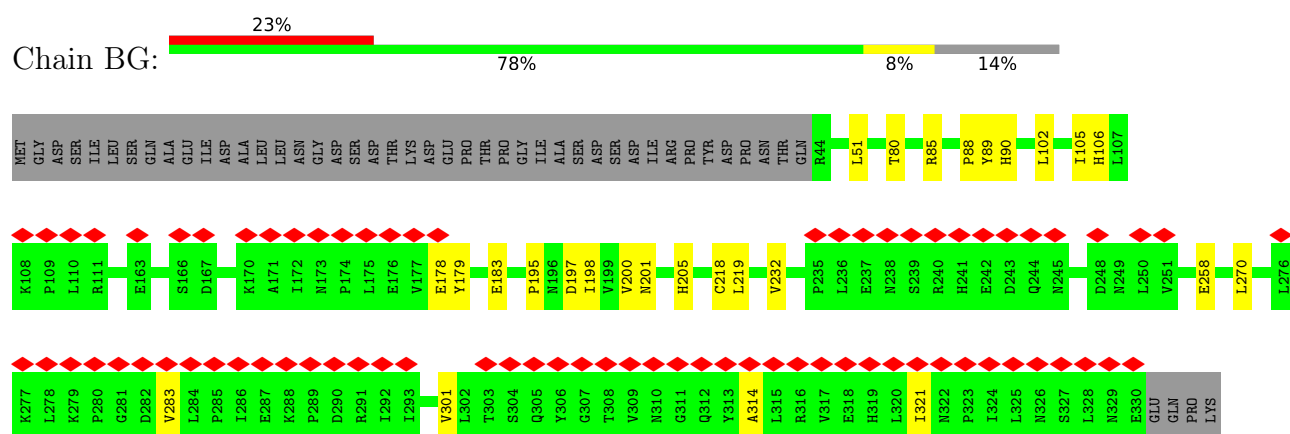
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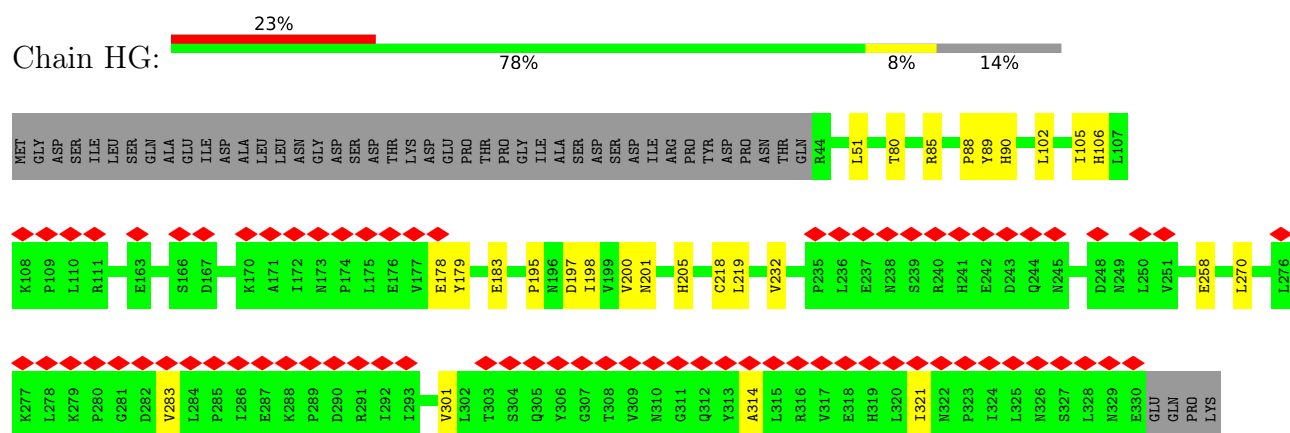
## ● Molecule 3: Flagellar motor switch protein FlIM



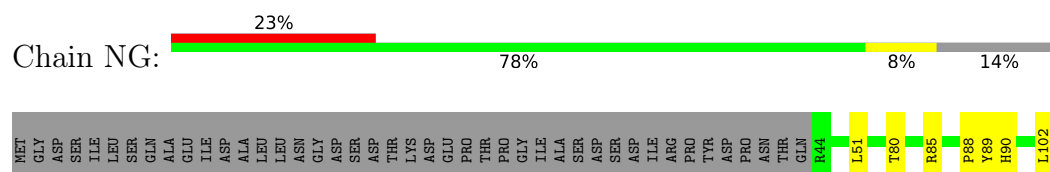
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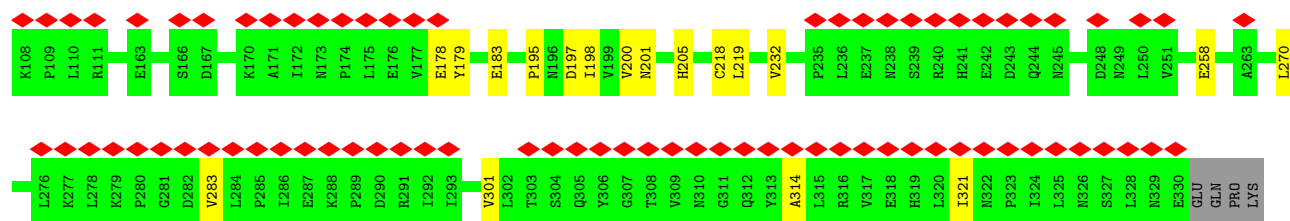


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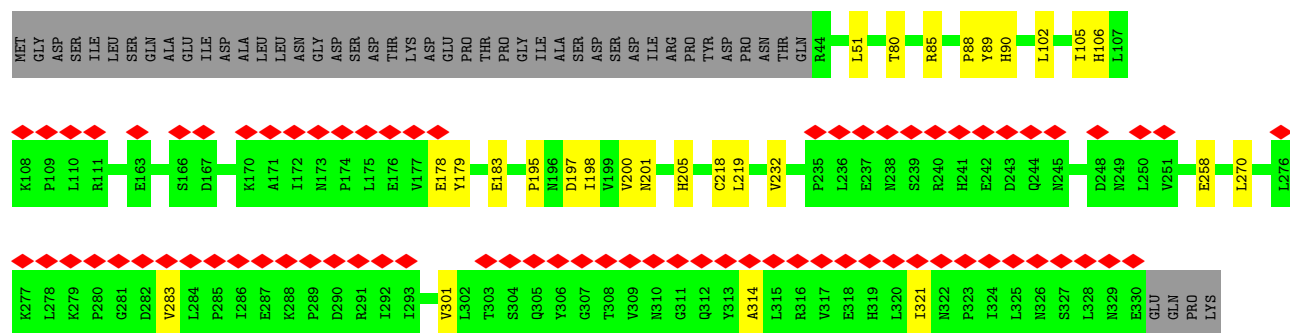
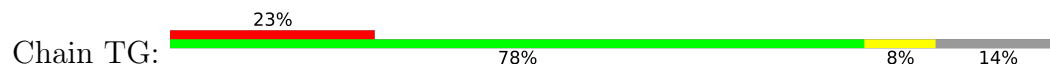


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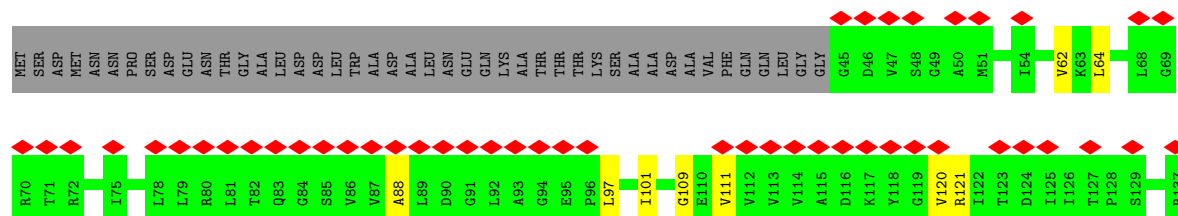




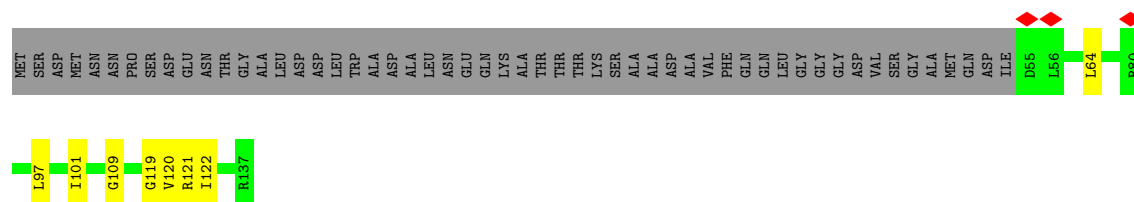
• Molecule 3: Flagellar motor switch protein FliM



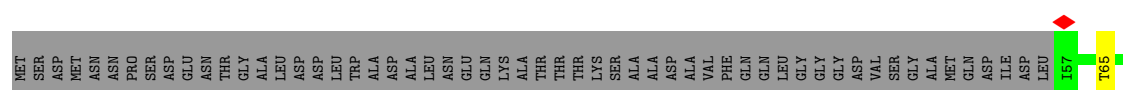
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

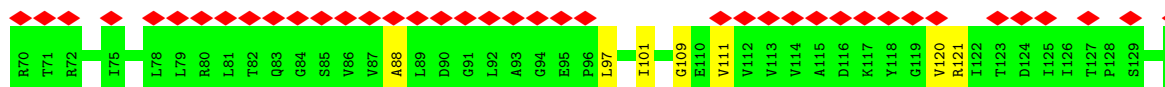
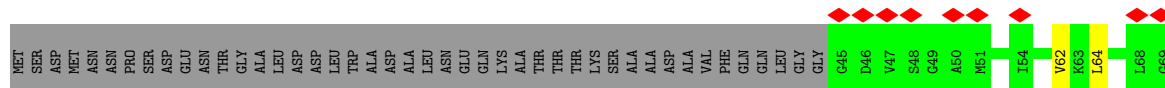


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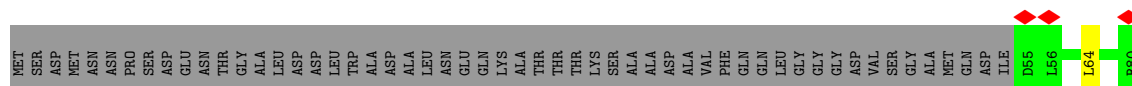




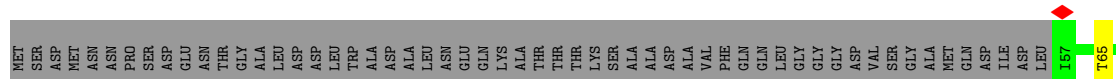
- Molecule 4: Flagellar motor switch protein FliN



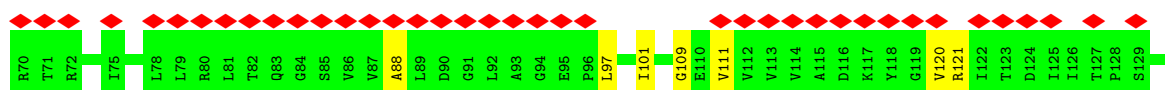
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- Molecule 4: Flagellar motor switch protein FliN

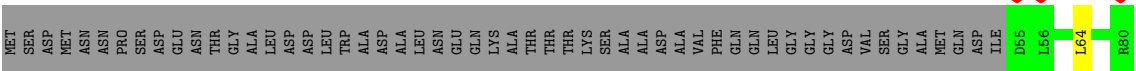


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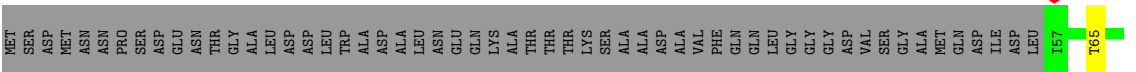


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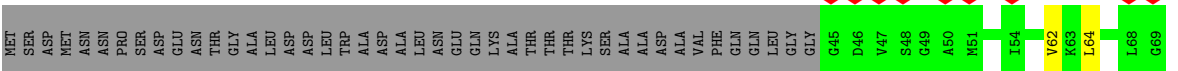




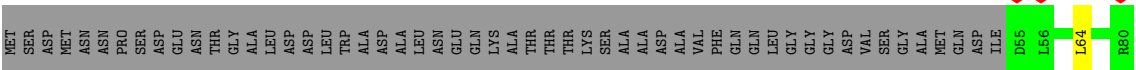
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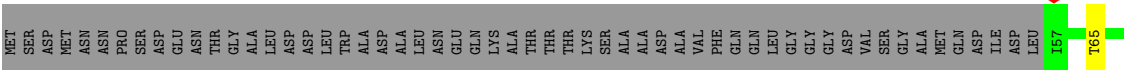
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

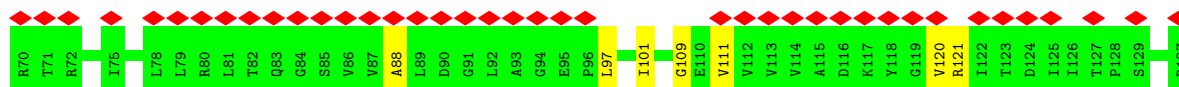
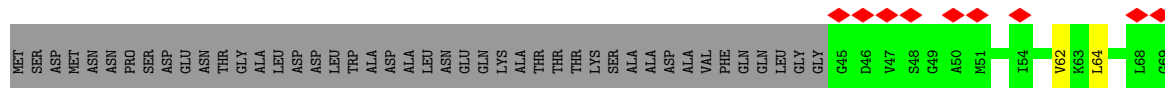
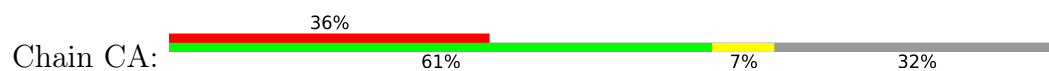


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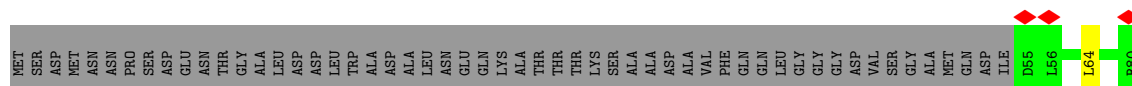




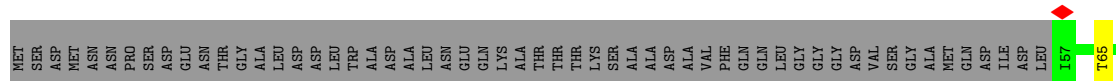
• Molecule 4: Flagellar motor switch protein FliN



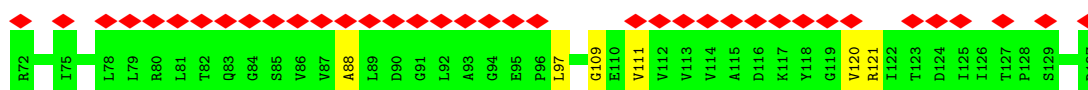
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

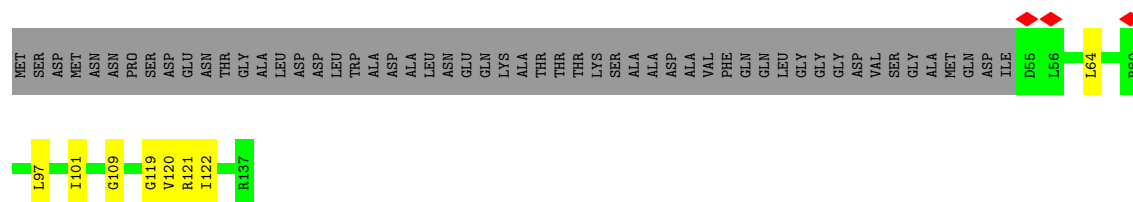


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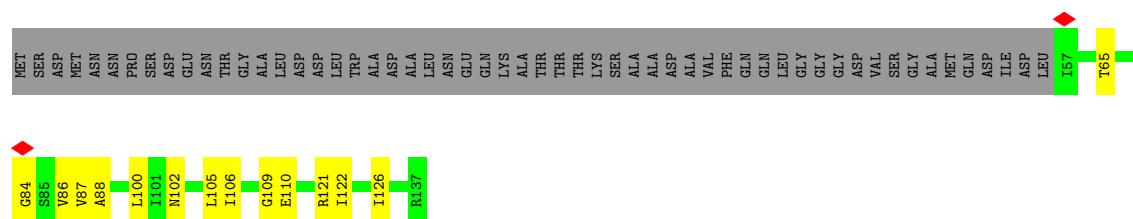
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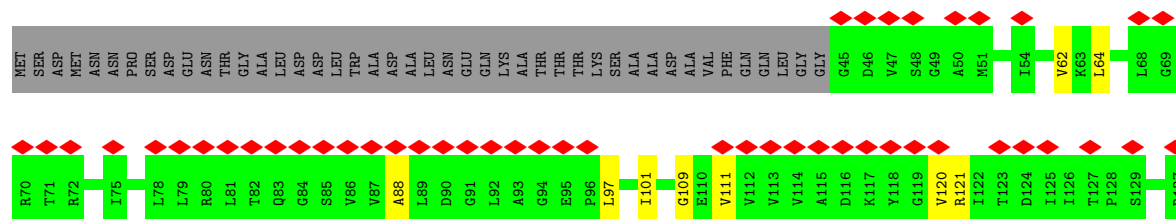
- Molecule 4: Flagellar motor switch protein FlhN

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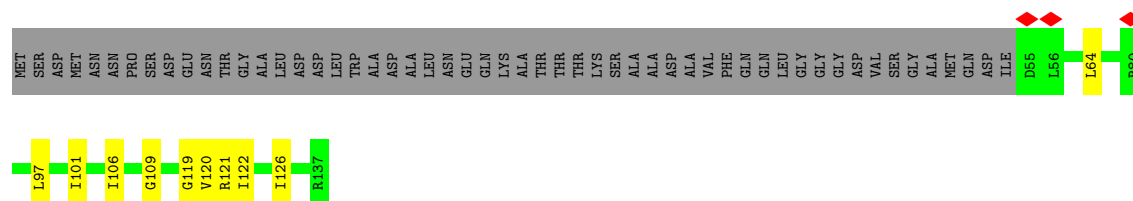
- Molecule 4: Flagellar motor switch protein FlhN

Chain OA: 



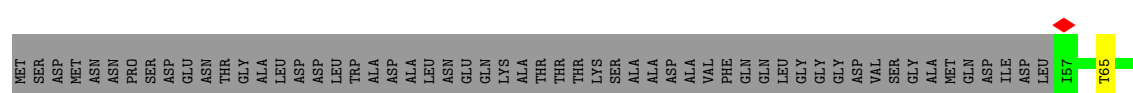
- Molecule 4: Flagellar motor switch protein FlhN

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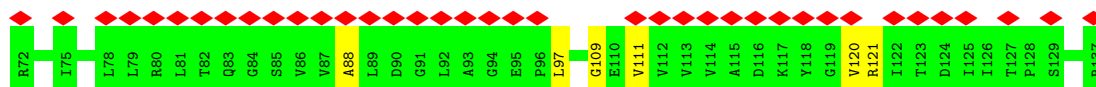
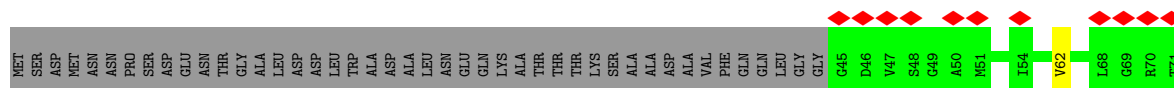
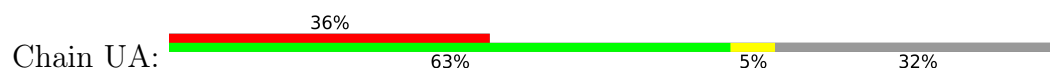
- Molecule 4: Flagellar motor switch protein FlhN

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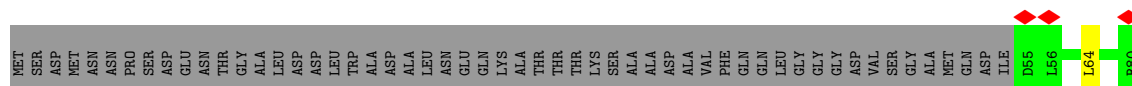




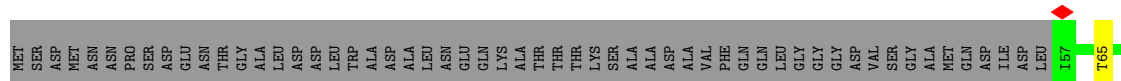
- Molecule 4: Flagellar motor switch protein FliN



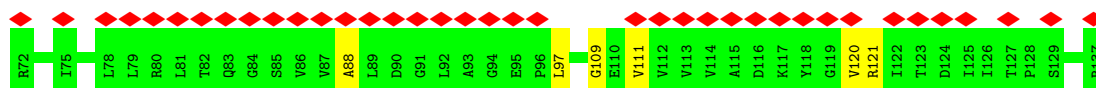
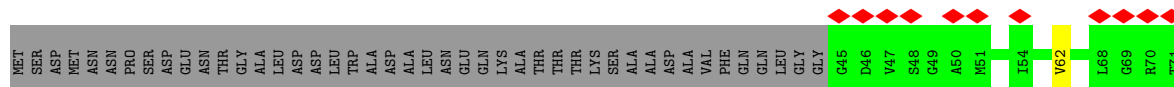
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

Sequence logo for the 100th position of the protein. The y-axis represents the frequency of amino acids, ranging from 0.00 to 0.10. The x-axis lists the amino acids. The 'L' residues (L97, I101, G109, G119, V120, R121, I122, R137) are highlighted in green, and the 'D' residues (D55, L56, L64, R60) are highlighted in red.

| Gene | Protein | Accession | Length (aa) | Weight (kDa) | PI   | Instability | Stability | Score | Rank |
|------|---------|-----------|-------------|--------------|------|-------------|-----------|-------|------|
| G84  | Met     | Met       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 1    |
| S85  | Ser     | Ser       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 2    |
| V86  | Asp     | Asp       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 3    |
| V87  | Met     | Met       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 4    |
| A88  | Asn     | Asn       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 5    |
| L100 | Pro     | Pro       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 6    |
| I101 | Ser     | Ser       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 7    |
| M102 | Asp     | Asp       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 8    |
| L105 | Asn     | Asn       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 9    |
| I106 | Thr     | Thr       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 10   |
| G109 | Gly     | Gly       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 11   |
| E110 | Ala     | Ala       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 12   |
| R121 | Asp     | Asp       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 13   |
| I122 | Leu     | Leu       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 14   |
| I126 | Trp     | Trp       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 15   |
| I137 | Ala     | Ala       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 16   |
| I137 | Asn     | Asn       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 17   |
| I137 | Glu     | Glu       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 18   |
| I137 | Gln     | Gln       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 19   |
| I137 | Lys     | Lys       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 20   |
| I137 | Thr     | Thr       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 21   |
| I137 | Thr     | Thr       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 22   |
| I137 | Lys     | Lys       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 23   |
| I137 | Ser     | Ser       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 24   |
| I137 | Ala     | Ala       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 25   |
| I137 | Ala     | Ala       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 26   |
| I137 | Val     | Val       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 27   |
| I137 | Phe     | Phe       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 28   |
| I137 | Gln     | Gln       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 29   |
| I137 | Gln     | Gln       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 30   |
| I137 | Leu     | Leu       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 31   |
| I137 | Gly     | Gly       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 32   |
| I137 | Gly     | Gly       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 33   |
| I137 | Asp     | Asp       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 34   |
| I137 | Val     | Val       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 35   |
| I137 | Ser     | Ser       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 36   |
| I137 | Gly     | Gly       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 37   |
| I137 | Ala     | Ala       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 38   |
| I137 | Met     | Met       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 39   |
| I137 | Gln     | Gln       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 40   |
| I137 | Asp     | Asp       | 1           | 0.005        | 5.00 | 0.00        | 0.00      | 0.00  | 41   |
| I137 | Ile     | Ile       | 1           | 0.005        |      |             |           |       |      |

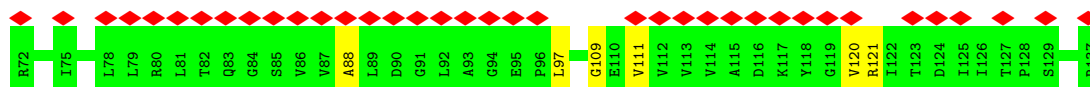
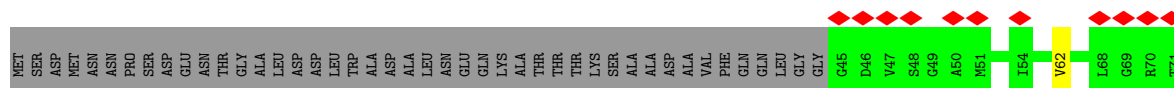
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|------|-----|-----|
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| I75  | Asp | Asp |
|      | Met | Met |
|      | Asn | Asn |
| L78  | Asn | Asn |
| L79  | Pro | Pro |
| R80  | Ser | Ser |
| L81  | Asp | Asp |
| T82  | Glu | Glu |
|      | Asn | Asn |
| Q83  | Thr | Thr |
| G84  | Gly | Gly |
| S85  | Ala | Ala |
| V86  | Leu | Leu |
| V87  | Asp | Asp |
|      | Asp | Asp |
| A88  | Leu | Leu |
|      | Trp | Trp |
| L89  | Ala | Ala |
| D90  | Ala | Ala |
| G91  | Ala | Ala |
| L92  | Leu | Leu |
| A93  | Asn | Asn |
| G94  | Glu | Glu |
| E95  | Gln | Gln |
| P96  | Lys | Lys |
|      | Ala | Ala |
| L97  | Ala | Ala |
|      | Thr | Thr |
|      | Thr | Thr |
| G109 | Lys | Lys |
| E110 | Ser | Ser |
| V111 | Ala | Ala |
|      | Ala | Ala |
| V112 | Asp | Asp |
| V113 | Ala | Ala |
| V114 | Ala | Ala |
| A115 | Val | Val |
| A116 | Phe | Phe |
| K117 | Gln | Gln |
| Y118 | Gln | Gln |
| G119 | Leu | Leu |
| V120 | Leu | Leu |
| R121 | Gly | Gly |
| I122 | Gly | Gly |
| T123 | G45 | G45 |
| D124 | D46 | D46 |
|      | V47 | V47 |
| D124 | S48 | S48 |
| I126 | G49 | G49 |
| T127 | A50 | A50 |
| P128 | M51 | M51 |
| S129 |     |     |
|      | I54 | I54 |
| R137 | V62 | V62 |
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|      | T71 | T71 |

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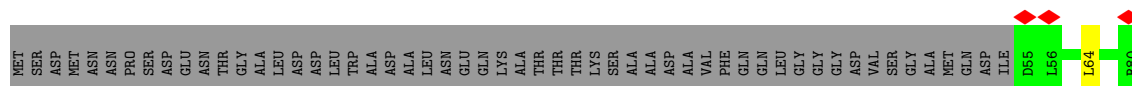
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | ASP | MET | ASN | ASN | PRO | SER | ASP | GLU | ASN | THR | GLY | LEU | ASP | ASP | LEU | TRP | ALA | ASP | ALA | ALA | LEU | ASN | GLU | GLN | LYS | ALA | THR | THR | THR | LYS | SER | ALA | ALA | ASP | ALA | VAL | PHE | GLN | GLN | LEU | GLY | GLY | GLY | ASP | VAL | SER | SER | GLY | ALA | MET | GLN | ASP | ILE | ASP | LEU | LEU | I57 | T65 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



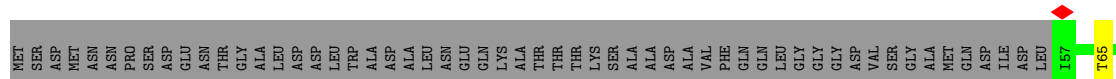
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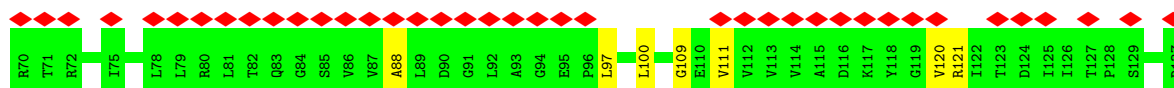
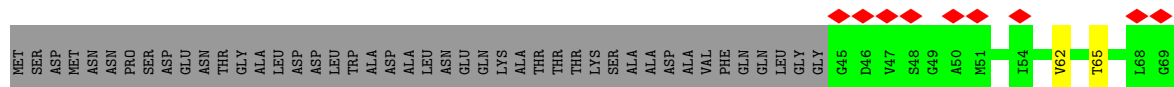
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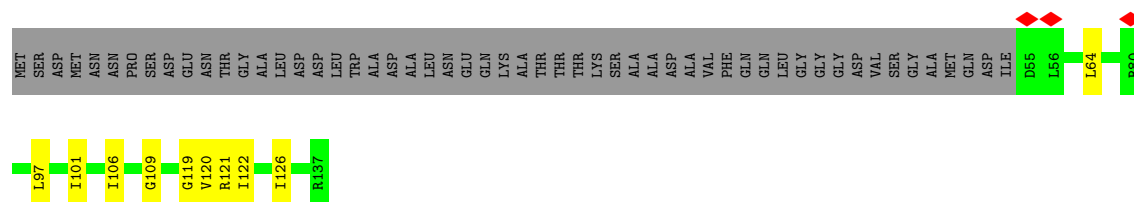
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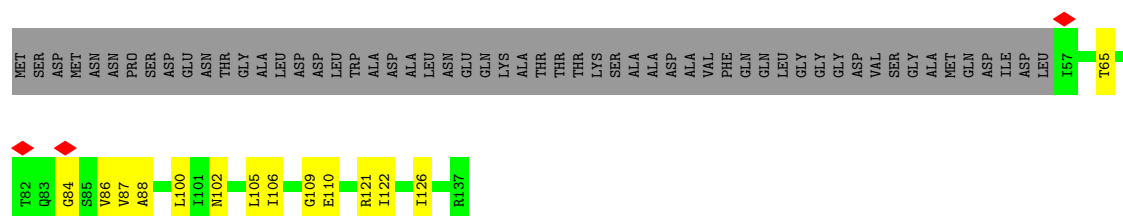
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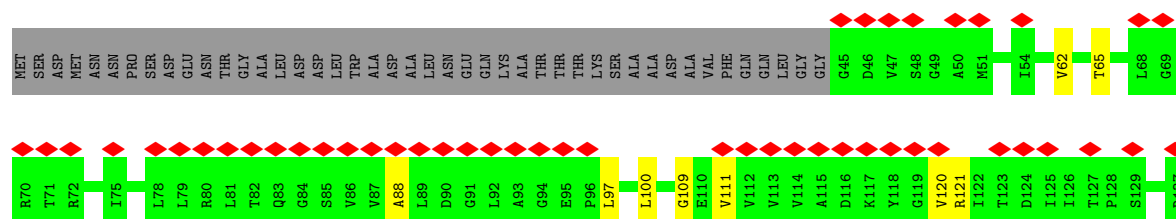
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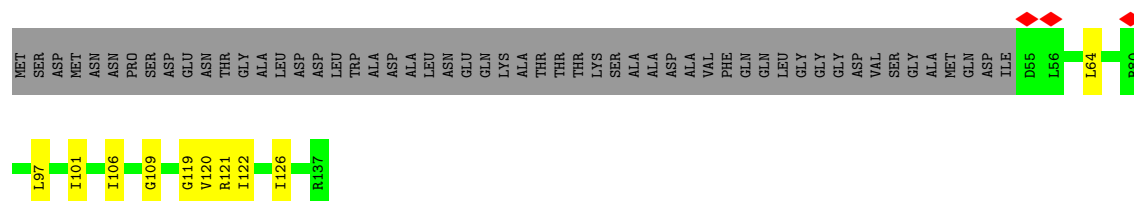
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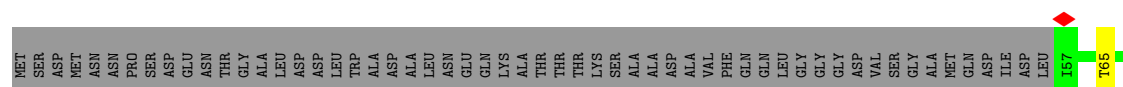
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• Molecule 4: Flagellar motor switch protein FliN

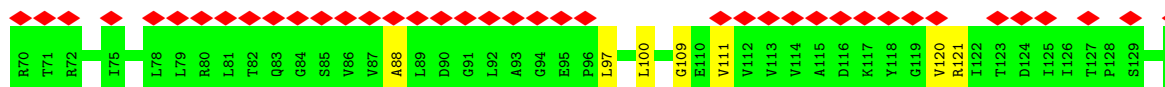
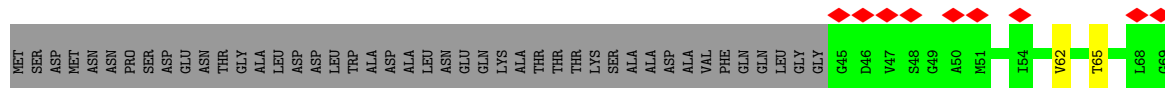


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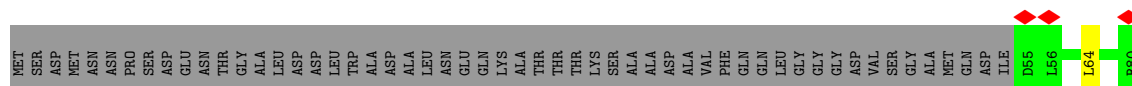




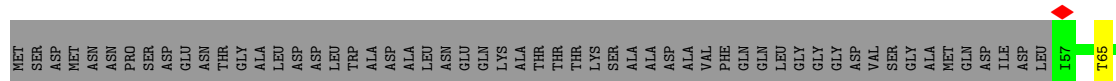
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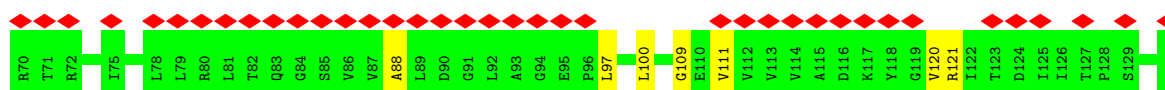
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- Molecule 4: Flagellar motor switch protein FliN

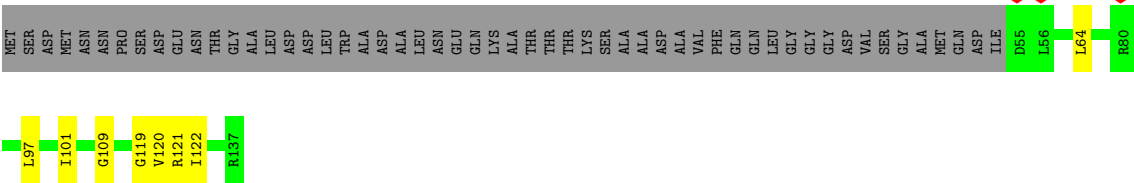


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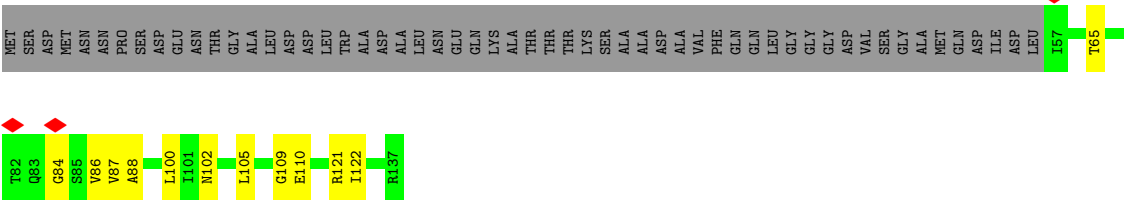


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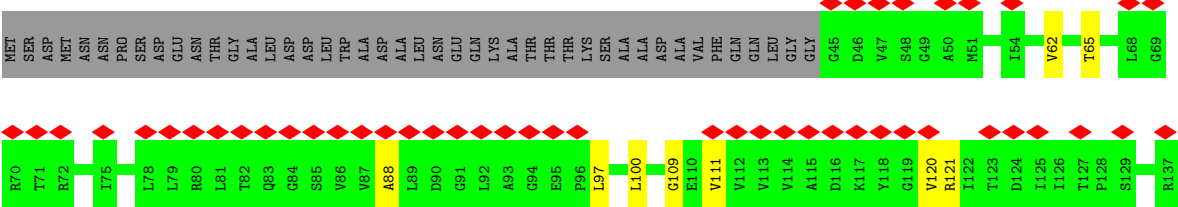




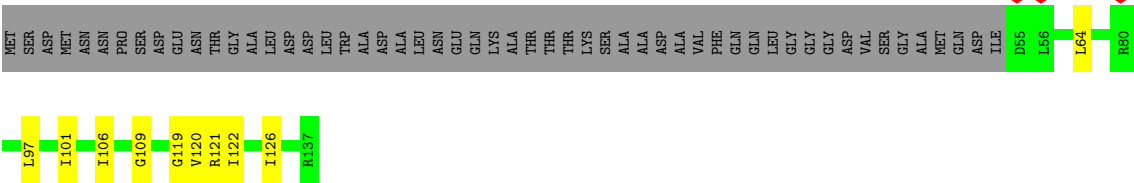
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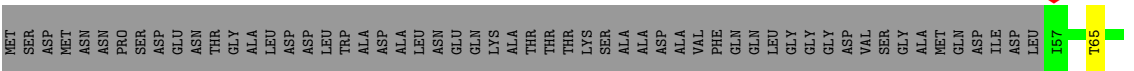
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• Molecule 4: Flagellar motor switch protein FliN

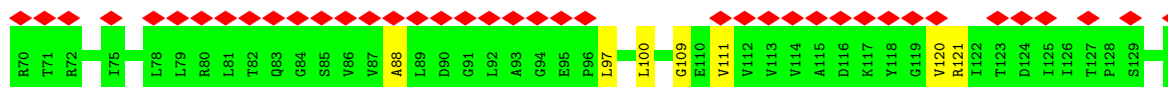
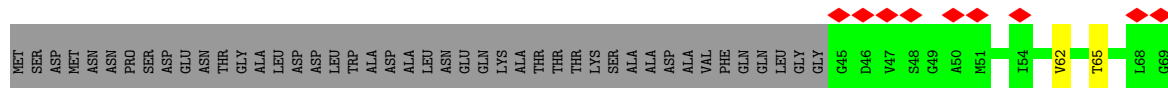


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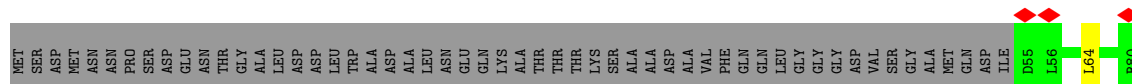




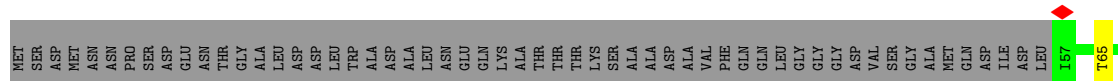
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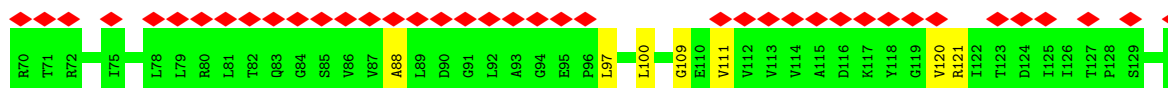
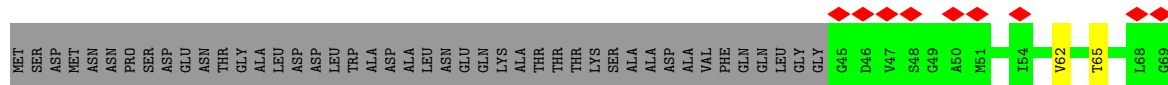
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- Molecule 4: Flagellar motor switch protein FliN

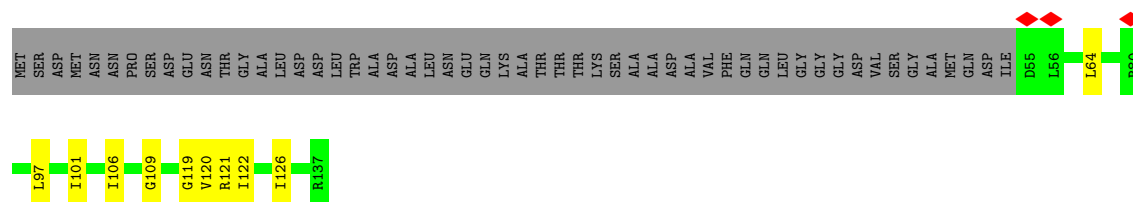


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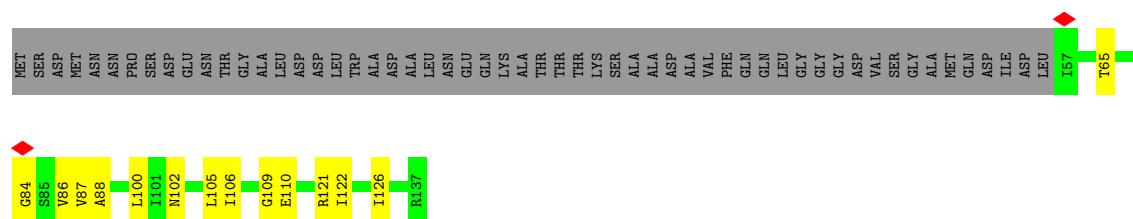
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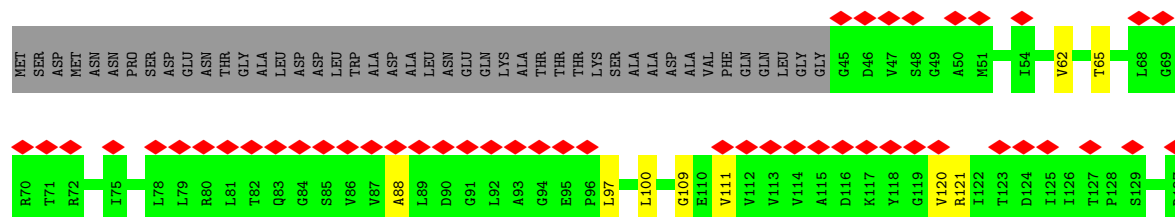
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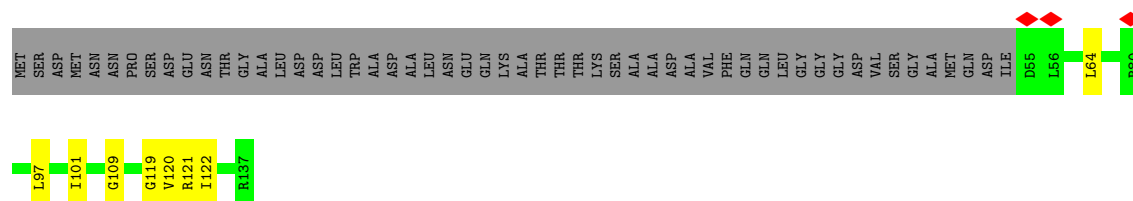
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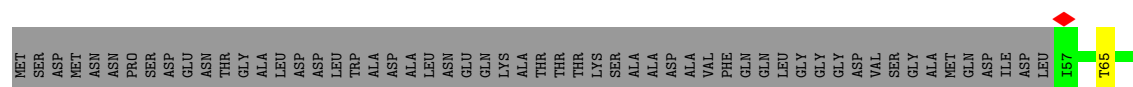
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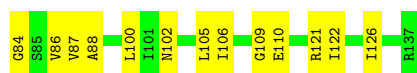
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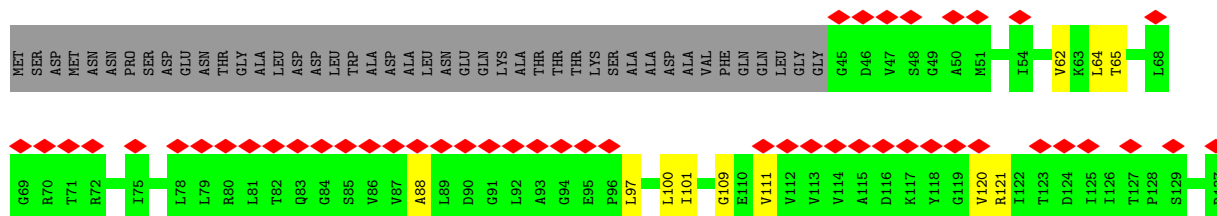
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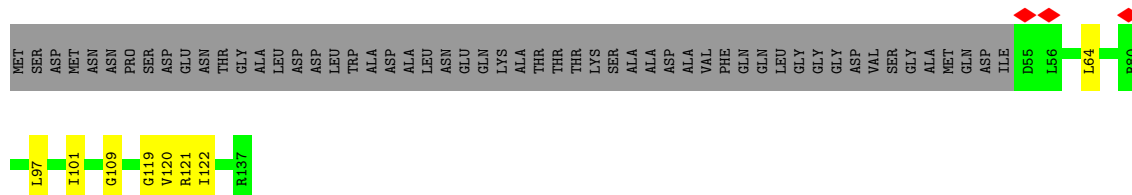




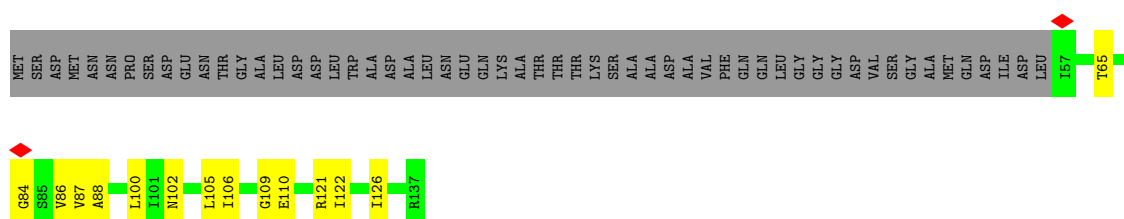
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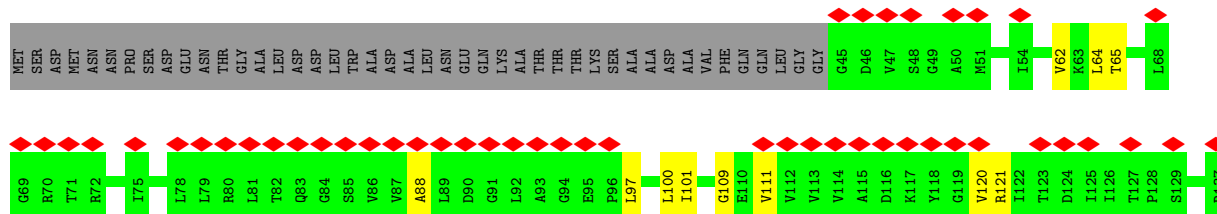
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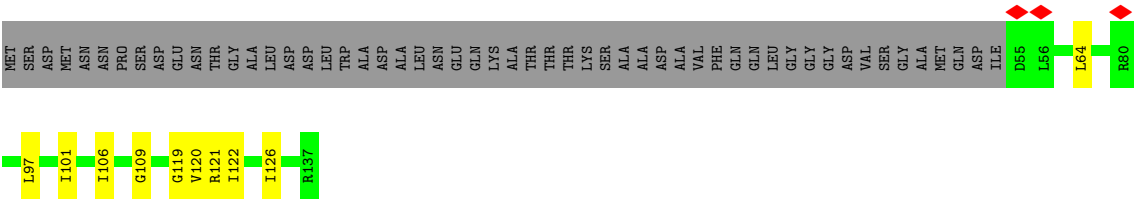
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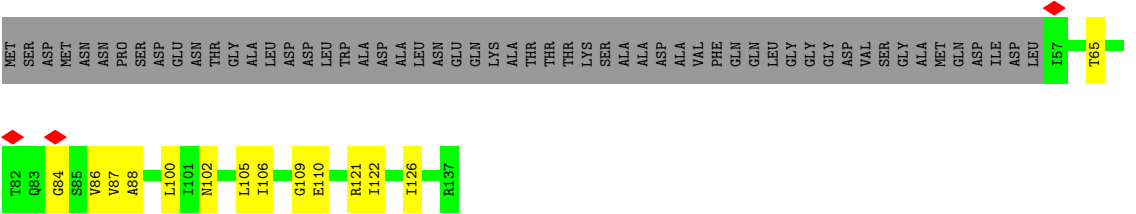
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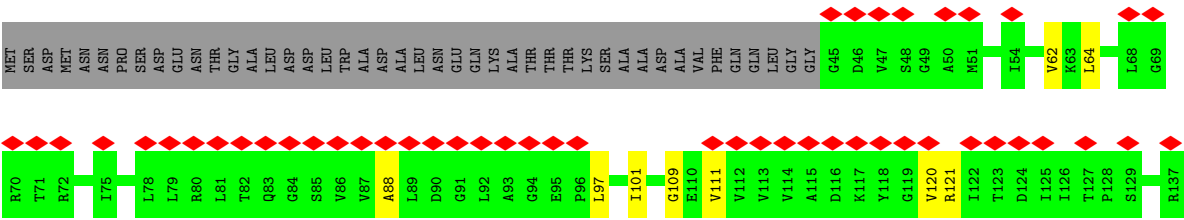
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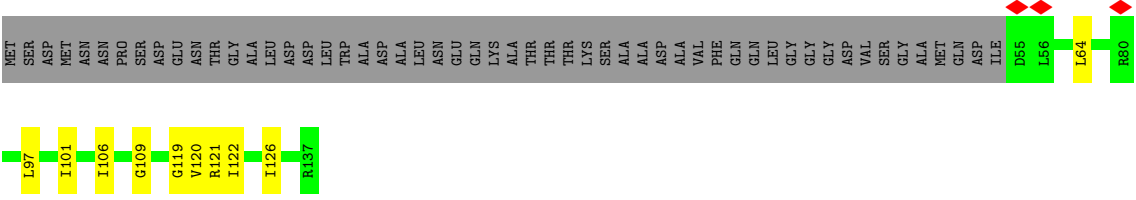
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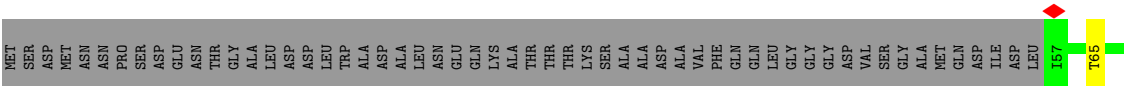
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• Molecule 4: Flagellar motor switch protein FliN

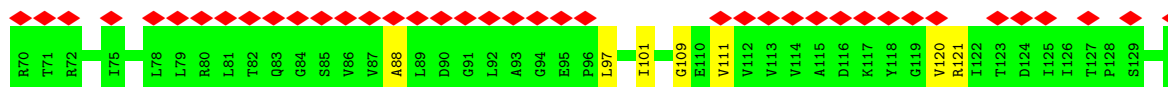
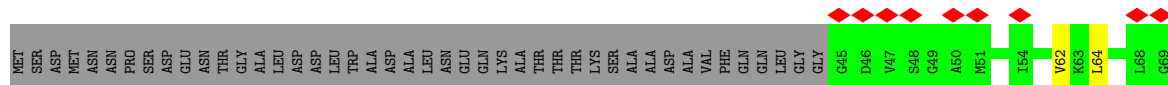


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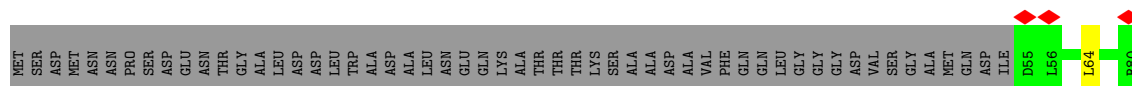




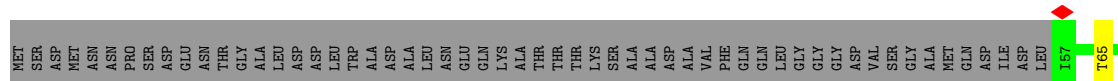
- Molecule 4: Flagellar motor switch protein FliN



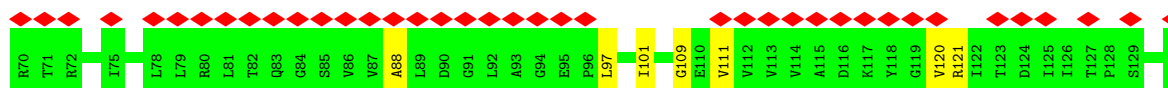
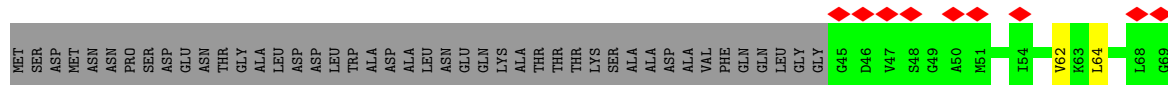
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- Molecule 4: Flagellar motor switch protein FliN

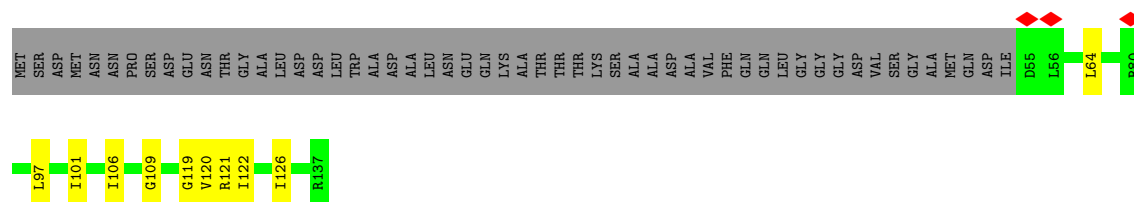


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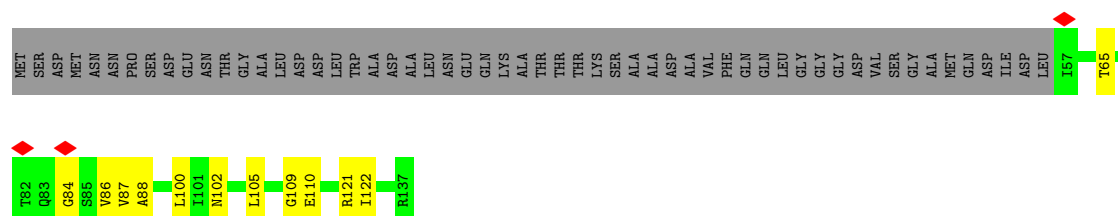
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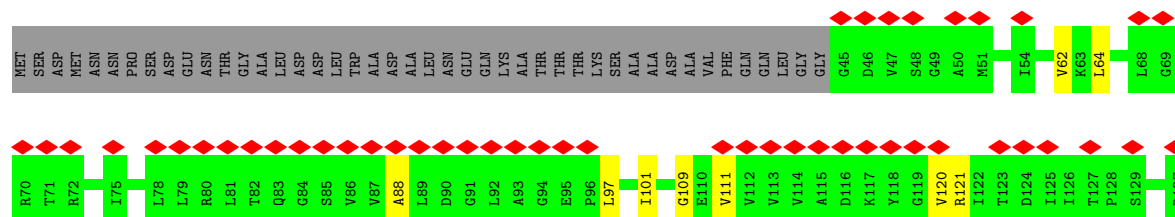
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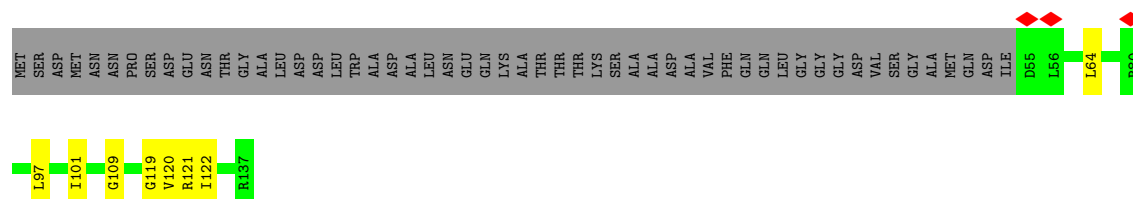
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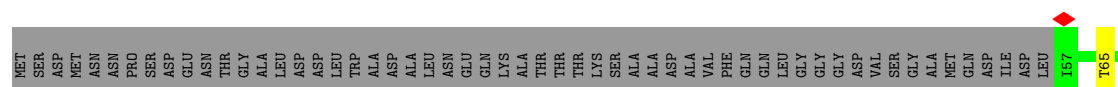
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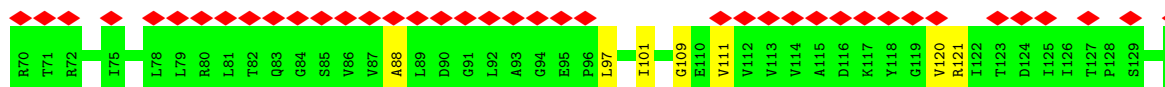
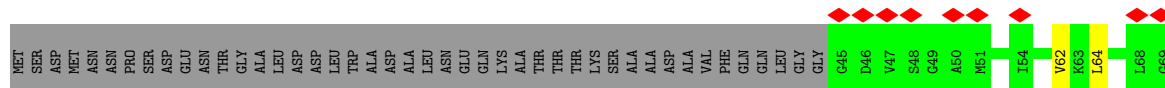
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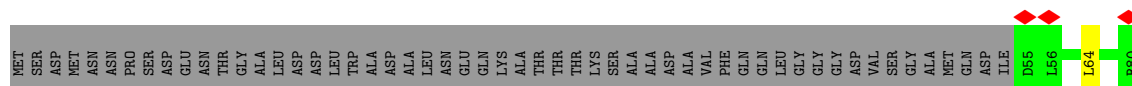




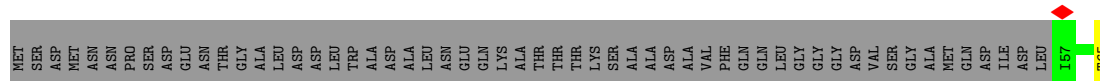
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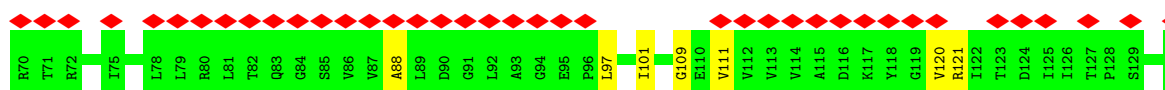
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- Molecule 4: Flagellar motor switch protein FliN



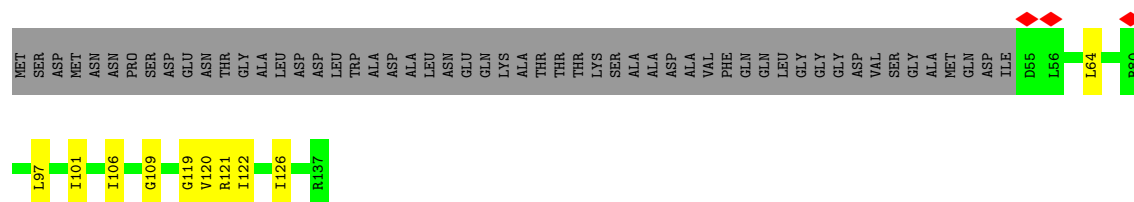
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- Molecule 4: Flagellar motor switch protein FliN

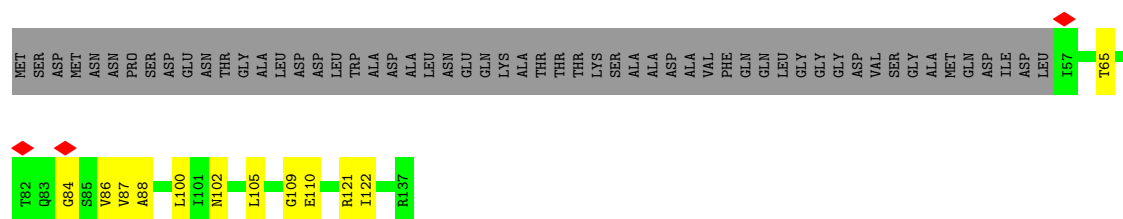


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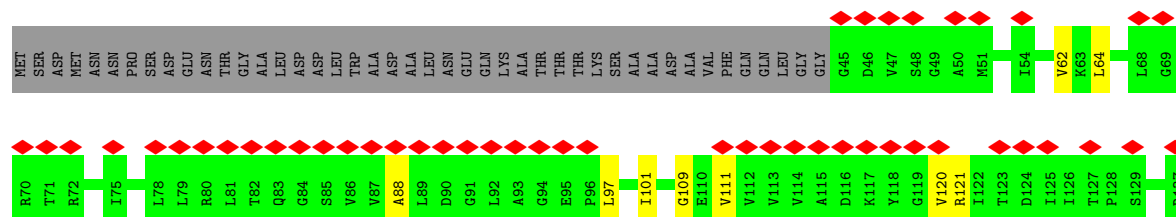
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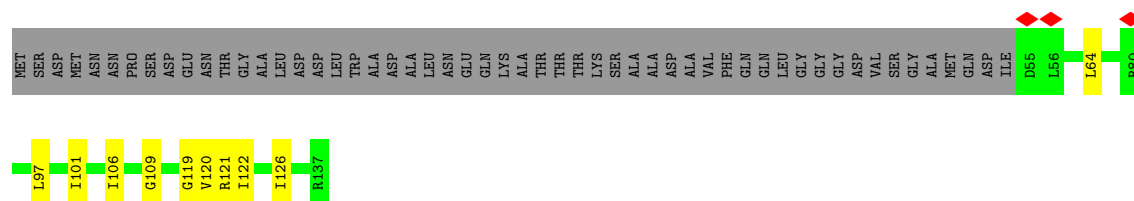
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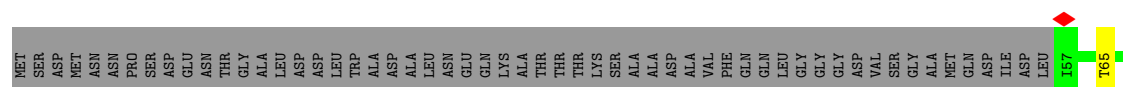
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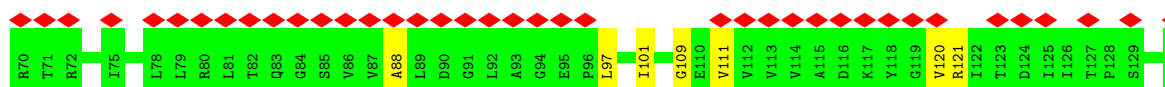
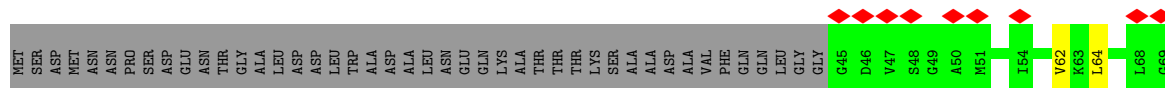
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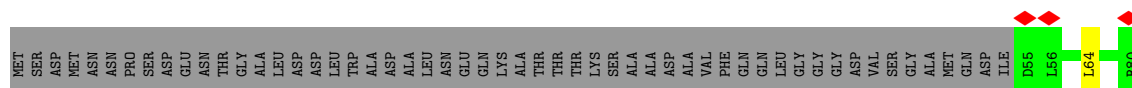




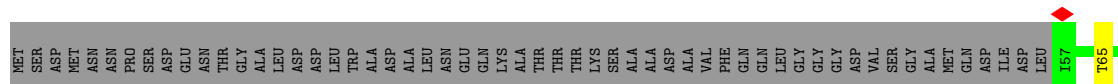
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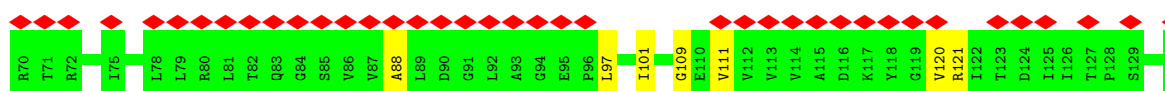
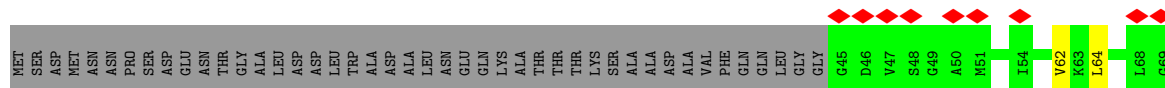
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- Molecule 4: Flagellar motor switch protein FliN

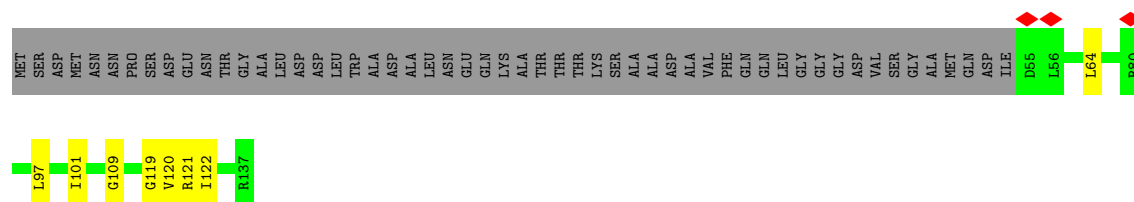


- Molecule 4: Flagellar motor switch protein FliN



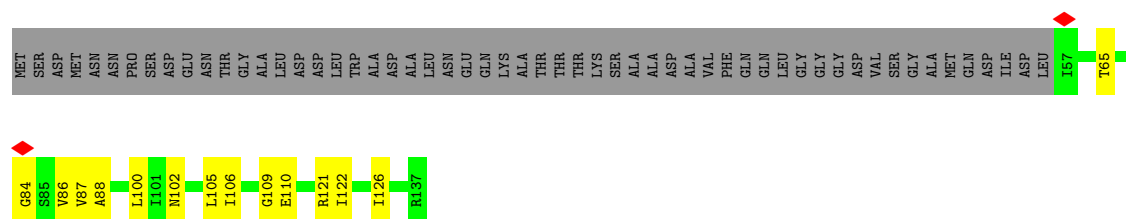
- Molecule 4: Flagellar motor switch protein FliN

Chain XF: 



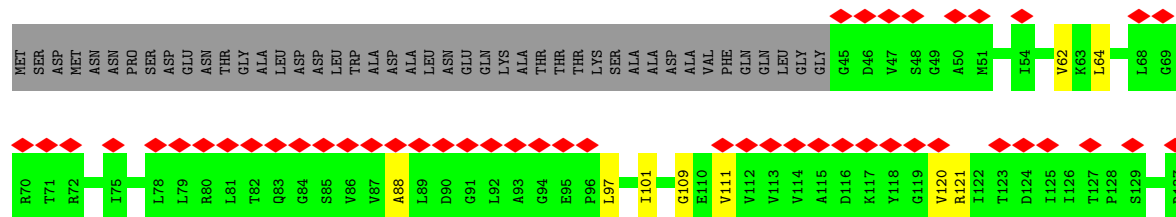
- Molecule 4: Flagellar motor switch protein FliN

Chain YF: 



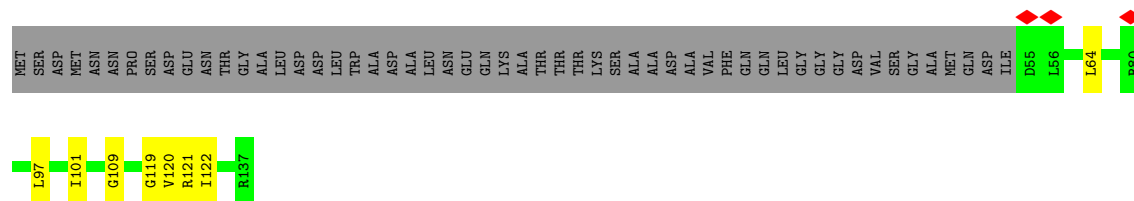
- Molecule 4: Flagellar motor switch protein FliN

Chain CG: 



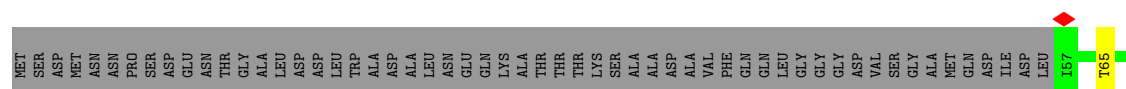
- Molecule 4: Flagellar motor switch protein FliN

Chain DG: 



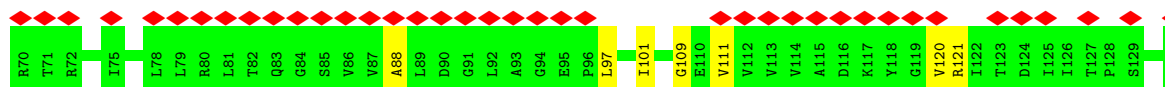
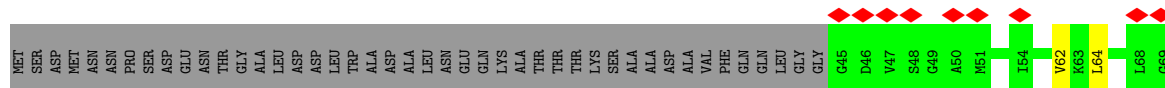
- Molecule 4: Flagellar motor switch protein FliN

Chain EG: 

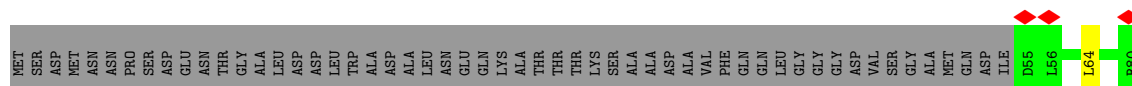




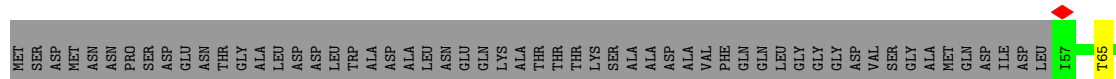
- Molecule 4: Flagellar motor switch protein FliN



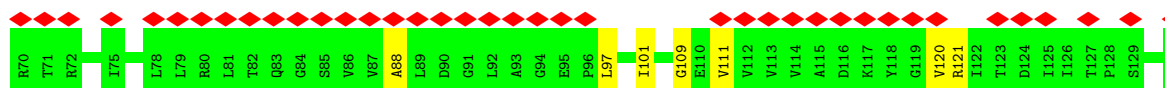
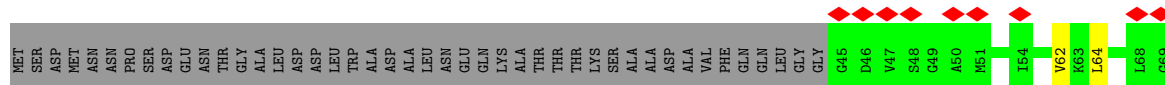
- Molecule 4: Flagellar motor switch protein FliN



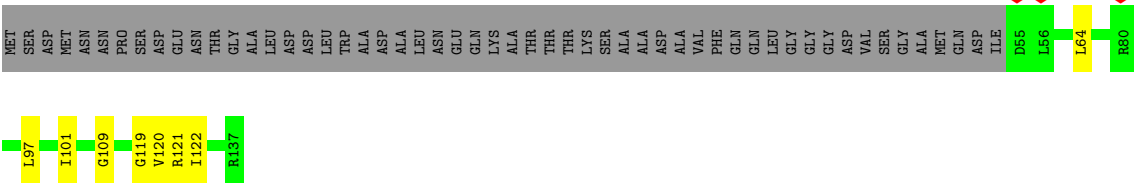
- Molecule 4: Flagellar motor switch protein FliN



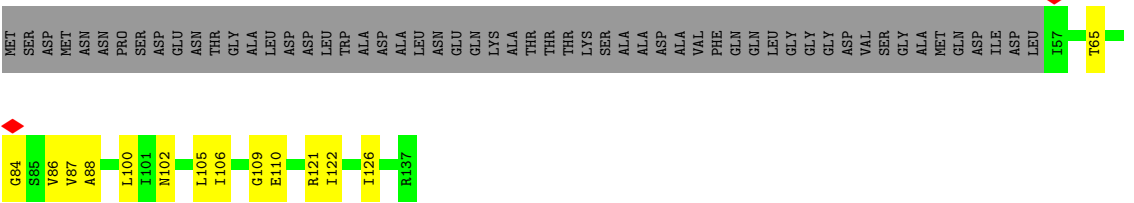
- Molecule 4: Flagellar motor switch protein FliN



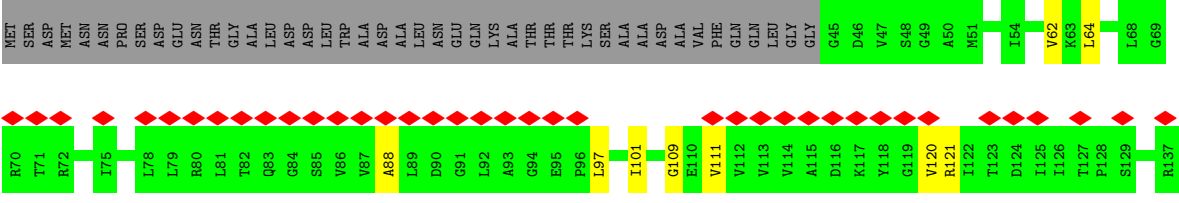
- Molecule 4: Flagellar motor switch protein FliN



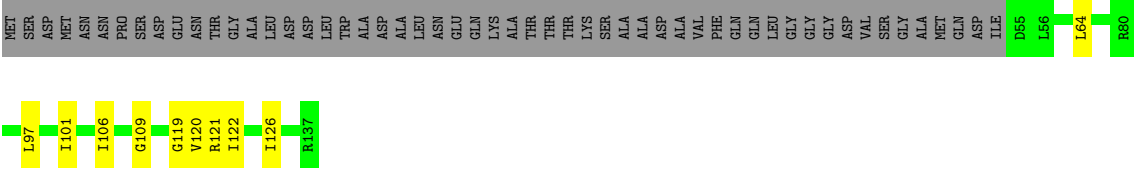
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

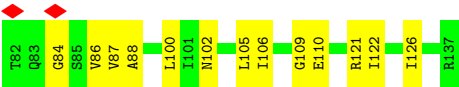


• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 11106                                   | 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 ( $e^-/\text{\AA}^2$ ) | 59.242                                  | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.283                                   | Depositor |
| Minimum map value                    | -0.060                                  | Depositor |
| Average map value                    | -0.001                                  | Depositor |
| Map value standard deviation         | 0.018                                   | Depositor |
| Recommended contour level            | 0.175                                   | Depositor |
| Map size (Å)                         | 1047.04, 1047.04, 1047.04               | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 2.045, 2.045, 2.045                     | 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     | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | BC    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | BF    | 1.03         | 0/233   | 1.26        | 0/324   |
| 1   | DB    | 1.02         | 0/233   | 1.26        | 0/324   |
| 1   | DE    | 1.03         | 0/233   | 1.25        | 0/324   |
| 1   | F     | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | FA    | 1.02         | 0/233   | 1.26        | 0/324   |
| 1   | FD    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | FG    | 1.02         | 0/233   | 1.26        | 0/324   |
| 1   | HC    | 1.03         | 0/233   | 1.26        | 0/324   |
| 1   | HF    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | I     | 1.02         | 0/233   | 1.26        | 0/324   |
| 1   | JB    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | JE    | 1.03         | 0/233   | 1.26        | 0/324   |
| 1   | LA    | 1.03         | 0/233   | 1.26        | 0/324   |
| 1   | LD    | 1.02         | 0/233   | 1.26        | 0/324   |
| 1   | LG    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | NC    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | NF    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | PB    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | PE    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | RA    | 1.03         | 0/233   | 1.26        | 0/324   |
| 1   | RD    | 1.03         | 0/233   | 1.25        | 0/324   |
| 1   | RG    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | S     | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | TC    | 1.03         | 0/233   | 1.25        | 0/324   |
| 1   | TF    | 1.03         | 0/233   | 1.25        | 0/324   |
| 1   | VB    | 1.03         | 0/233   | 1.25        | 0/324   |
| 1   | VE    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | XA    | 1.03         | 0/233   | 1.25        | 0/324   |
| 1   | XD    | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | Z     | 1.02         | 0/233   | 1.25        | 0/324   |
| 1   | ZC    | 1.03         | 0/233   | 1.25        | 0/324   |
| 1   | ZF    | 1.03         | 0/233   | 1.26        | 0/324   |



| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 2   | AA    | 0.72         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | AD    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | AG    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | B     | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | CC    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | CF    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | EB    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | EE    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | G     | 0.71         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | GA    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | GD    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | GG    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | IC    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | IF    | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | J     | 0.71         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | KB    | 0.72         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | KE    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | MA    | 0.72         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | MD    | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | MG    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | OC    | 0.71         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | OF    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | QB    | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | QE    | 0.71         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | SA    | 0.71         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | SD    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | SG    | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | T     | 0.72         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | UC    | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | UF    | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | WB    | 0.71         | 1/1577 (0.1%) | 0.92        | 5/2195 (0.2%) |
| 2   | WE    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | YA    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 2   | YD    | 0.72         | 1/1577 (0.1%) | 0.93        | 5/2195 (0.2%) |
| 3   | BA    | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | BD    | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | BG    | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | C     | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | DC    | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | DF    | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | FB    | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | FE    | 0.40         | 0/1419        | 0.54        | 0/1976        |
| 3   | HA    | 0.40         | 0/1419        | 0.54        | 0/1976        |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 3   | HD    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | HG    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | JC    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | JF    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | K     | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | LB    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | LE    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | M     | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | NA    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | ND    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | NG    | 0.40         | 0/1419  | 0.55        | 0/1976  |
| 3   | PC    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | PF    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | RB    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | RE    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | TA    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | TD    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | TG    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | V     | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | VC    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | VF    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | XB    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | XE    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | ZA    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 3   | ZD    | 0.40         | 0/1419  | 0.54        | 0/1976  |
| 4   | AB    | 0.56         | 0/455   | 0.65        | 0/630   |
| 4   | AC    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | AE    | 0.56         | 0/455   | 0.65        | 0/630   |
| 4   | AF    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | BB    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | BE    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | CA    | 0.56         | 0/455   | 0.65        | 0/630   |
| 4   | CB    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | CD    | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | CE    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | CG    | 0.56         | 0/455   | 0.66        | 0/630   |
| 4   | D     | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | DA    | 0.40         | 0/408   | 0.48        | 0/564   |
| 4   | DD    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | DG    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | E     | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | EA    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | EC    | 0.56         | 0/455   | 0.66        | 0/630   |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 4   | ED    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | EF    | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | EG    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | FC    | 0.40         | 0/408   | 0.48        | 0/564   |
| 4   | FF    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | GB    | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | GC    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | GE    | 0.56         | 0/455   | 0.65        | 0/630   |
| 4   | GF    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | H     | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | HB    | 0.40         | 0/408   | 0.48        | 0/564   |
| 4   | HE    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | IA    | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | IB    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | ID    | 0.55         | 0/455   | 0.66        | 0/630   |
| 4   | IE    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | IG    | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | JA    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | JD    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | JG    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | KA    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | KC    | 0.55         | 0/455   | 0.66        | 0/630   |
| 4   | KD    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | KF    | 0.55         | 0/455   | 0.66        | 0/630   |
| 4   | KG    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | L     | 0.56         | 0/455   | 0.66        | 0/630   |
| 4   | LC    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | LF    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | MB    | 0.56         | 0/455   | 0.65        | 0/630   |
| 4   | MC    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | ME    | 0.56         | 0/455   | 0.65        | 0/630   |
| 4   | MF    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | N     | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | NB    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | NE    | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | O     | 0.40         | 0/408   | 0.48        | 0/564   |
| 4   | OA    | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | OB    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | OD    | 0.55         | 0/455   | 0.65        | 0/630   |
| 4   | OE    | 0.31         | 0/398   | 0.42        | 0/550   |
| 4   | OG    | 0.55         | 0/455   | 0.66        | 0/630   |
| 4   | P     | 0.40         | 0/408   | 0.49        | 0/564   |
| 4   | PA    | 0.40         | 0/408   | 0.49        | 0/564   |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 4   | PD    | 0.40         | 0/408            | 0.48        | 0/564             |
| 4   | PG    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | Q     | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | QA    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | QC    | 0.56         | 0/455            | 0.65        | 0/630             |
| 4   | QD    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | QF    | 0.56         | 0/455            | 0.65        | 0/630             |
| 4   | QG    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | R     | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | RC    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | RF    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | SB    | 0.56         | 0/455            | 0.65        | 0/630             |
| 4   | SC    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | SE    | 0.56         | 0/455            | 0.65        | 0/630             |
| 4   | SF    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | TB    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | TE    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | UA    | 0.55         | 0/455            | 0.65        | 0/630             |
| 4   | UB    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | UD    | 0.56         | 0/455            | 0.65        | 0/630             |
| 4   | UE    | 0.30         | 0/398            | 0.42        | 0/550             |
| 4   | UG    | 0.55         | 0/455            | 0.65        | 0/630             |
| 4   | VA    | 0.40         | 0/408            | 0.48        | 0/564             |
| 4   | VD    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | VG    | 0.40         | 0/408            | 0.48        | 0/564             |
| 4   | W     | 0.56         | 0/455            | 0.65        | 0/630             |
| 4   | WA    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | WC    | 0.55         | 0/455            | 0.65        | 0/630             |
| 4   | WD    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | WF    | 0.55         | 0/455            | 0.65        | 0/630             |
| 4   | WG    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | X     | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | XC    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | XF    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | Y     | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | YB    | 0.56         | 0/455            | 0.66        | 0/630             |
| 4   | YC    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | YE    | 0.56         | 0/455            | 0.66        | 0/630             |
| 4   | YF    | 0.31         | 0/398            | 0.42        | 0/550             |
| 4   | ZB    | 0.40         | 0/408            | 0.49        | 0/564             |
| 4   | ZE    | 0.40         | 0/408            | 0.49        | 0/564             |
| All | All   | 0.58         | 34/152660 (0.0%) | 0.75        | 170/212126 (0.1%) |

All (34) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | SG    | 207 | LYS  | C-N   | -6.61 | 1.25        | 1.33     |
| 2   | CC    | 207 | LYS  | C-N   | -6.59 | 1.25        | 1.33     |
| 2   | AG    | 207 | LYS  | C-N   | -6.59 | 1.25        | 1.33     |
| 2   | GD    | 207 | LYS  | C-N   | -6.59 | 1.25        | 1.33     |
| 2   | YA    | 207 | LYS  | C-N   | -6.58 | 1.25        | 1.33     |
| 2   | WE    | 207 | LYS  | C-N   | -6.58 | 1.25        | 1.33     |
| 2   | AA    | 207 | LYS  | C-N   | -6.58 | 1.25        | 1.33     |
| 2   | UC    | 207 | LYS  | C-N   | -6.58 | 1.25        | 1.33     |
| 2   | EE    | 207 | LYS  | C-N   | -6.58 | 1.25        | 1.33     |
| 2   | T     | 207 | LYS  | C-N   | -6.57 | 1.25        | 1.33     |
| 2   | QB    | 207 | LYS  | C-N   | -6.57 | 1.25        | 1.33     |
| 2   | IC    | 207 | LYS  | C-N   | -6.57 | 1.25        | 1.33     |
| 2   | GG    | 207 | LYS  | C-N   | -6.57 | 1.25        | 1.33     |
| 2   | KB    | 207 | LYS  | C-N   | -6.56 | 1.25        | 1.33     |
| 2   | QE    | 207 | LYS  | C-N   | -6.55 | 1.25        | 1.33     |
| 2   | B     | 207 | LYS  | C-N   | -6.55 | 1.25        | 1.33     |
| 2   | OC    | 207 | LYS  | C-N   | -6.55 | 1.25        | 1.33     |
| 2   | MD    | 207 | LYS  | C-N   | -6.55 | 1.25        | 1.33     |
| 2   | MG    | 207 | LYS  | C-N   | -6.55 | 1.25        | 1.33     |
| 2   | EB    | 207 | LYS  | C-N   | -6.54 | 1.25        | 1.33     |
| 2   | G     | 207 | LYS  | C-N   | -6.53 | 1.25        | 1.33     |
| 2   | MA    | 207 | LYS  | C-N   | -6.53 | 1.25        | 1.33     |
| 2   | AD    | 207 | LYS  | C-N   | -6.53 | 1.25        | 1.33     |
| 2   | SD    | 207 | LYS  | C-N   | -6.53 | 1.25        | 1.33     |
| 2   | YD    | 207 | LYS  | C-N   | -6.53 | 1.25        | 1.33     |
| 2   | KE    | 207 | LYS  | C-N   | -6.53 | 1.25        | 1.33     |
| 2   | GA    | 207 | LYS  | C-N   | -6.53 | 1.25        | 1.33     |
| 2   | OF    | 207 | LYS  | C-N   | -6.52 | 1.25        | 1.33     |
| 2   | SA    | 207 | LYS  | C-N   | -6.52 | 1.25        | 1.33     |
| 2   | IF    | 207 | LYS  | C-N   | -6.51 | 1.25        | 1.33     |
| 2   | WB    | 207 | LYS  | C-N   | -6.51 | 1.25        | 1.33     |
| 2   | CF    | 207 | LYS  | C-N   | -6.51 | 1.25        | 1.33     |
| 2   | UF    | 207 | LYS  | C-N   | -6.51 | 1.25        | 1.33     |
| 2   | J     | 207 | LYS  | C-N   | -6.49 | 1.25        | 1.33     |

All (170) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | IC    | 186 | GLN  | N-CA-C | -7.41 | 103.38      | 114.64   |
| 2   | SG    | 186 | GLN  | N-CA-C | -7.40 | 103.39      | 114.64   |
| 2   | UC    | 186 | GLN  | N-CA-C | -7.38 | 103.42      | 114.64   |
| 2   | SD    | 186 | GLN  | N-CA-C | -7.38 | 103.43      | 114.64   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | YA    | 186 | GLN  | N-CA-C | -7.37 | 103.43      | 114.64   |
| 2   | WE    | 186 | GLN  | N-CA-C | -7.37 | 103.44      | 114.64   |
| 2   | B     | 186 | GLN  | N-CA-C | -7.37 | 103.44      | 114.64   |
| 2   | GA    | 186 | GLN  | N-CA-C | -7.37 | 103.45      | 114.64   |
| 2   | OC    | 186 | GLN  | N-CA-C | -7.37 | 103.44      | 114.64   |
| 2   | EE    | 186 | GLN  | N-CA-C | -7.37 | 103.45      | 114.64   |
| 2   | IF    | 186 | GLN  | N-CA-C | -7.37 | 103.44      | 114.64   |
| 2   | MG    | 186 | GLN  | N-CA-C | -7.37 | 103.44      | 114.64   |
| 2   | AA    | 186 | GLN  | N-CA-C | -7.36 | 103.45      | 114.64   |
| 2   | QB    | 186 | GLN  | N-CA-C | -7.36 | 103.45      | 114.64   |
| 2   | AD    | 186 | GLN  | N-CA-C | -7.36 | 103.45      | 114.64   |
| 2   | UF    | 186 | GLN  | N-CA-C | -7.36 | 103.45      | 114.64   |
| 2   | MA    | 186 | GLN  | N-CA-C | -7.36 | 103.45      | 114.64   |
| 2   | KE    | 186 | GLN  | N-CA-C | -7.36 | 103.45      | 114.64   |
| 2   | CF    | 186 | GLN  | N-CA-C | -7.36 | 103.46      | 114.64   |
| 2   | QE    | 186 | GLN  | N-CA-C | -7.35 | 103.46      | 114.64   |
| 2   | T     | 186 | GLN  | N-CA-C | -7.35 | 103.46      | 114.64   |
| 2   | GD    | 186 | GLN  | N-CA-C | -7.35 | 103.47      | 114.64   |
| 2   | AG    | 186 | GLN  | N-CA-C | -7.35 | 103.47      | 114.64   |
| 2   | GG    | 186 | GLN  | N-CA-C | -7.35 | 103.47      | 114.64   |
| 2   | CC    | 186 | GLN  | N-CA-C | -7.35 | 103.47      | 114.64   |
| 2   | WB    | 186 | GLN  | N-CA-C | -7.34 | 103.48      | 114.64   |
| 2   | J     | 186 | GLN  | N-CA-C | -7.34 | 103.49      | 114.64   |
| 2   | EB    | 186 | GLN  | N-CA-C | -7.34 | 103.49      | 114.64   |
| 2   | G     | 186 | GLN  | N-CA-C | -7.33 | 103.49      | 114.64   |
| 2   | YD    | 186 | GLN  | N-CA-C | -7.33 | 103.49      | 114.64   |
| 2   | OF    | 186 | GLN  | N-CA-C | -7.33 | 103.50      | 114.64   |
| 2   | MD    | 186 | GLN  | N-CA-C | -7.33 | 103.50      | 114.64   |
| 2   | SA    | 186 | GLN  | N-CA-C | -7.32 | 103.51      | 114.64   |
| 2   | KB    | 186 | GLN  | N-CA-C | -7.32 | 103.51      | 114.64   |
| 2   | KE    | 192 | LYS  | N-CA-C | -6.83 | 104.90      | 113.23   |
| 2   | G     | 192 | LYS  | N-CA-C | -6.82 | 104.91      | 113.23   |
| 2   | AD    | 192 | LYS  | N-CA-C | -6.82 | 104.91      | 113.23   |
| 2   | UC    | 192 | LYS  | N-CA-C | -6.82 | 104.92      | 113.23   |
| 2   | CF    | 192 | LYS  | N-CA-C | -6.81 | 104.92      | 113.23   |
| 2   | MD    | 192 | LYS  | N-CA-C | -6.81 | 104.92      | 113.23   |
| 2   | IC    | 192 | LYS  | N-CA-C | -6.80 | 104.93      | 113.23   |
| 2   | SG    | 192 | LYS  | N-CA-C | -6.80 | 104.93      | 113.23   |
| 2   | KB    | 192 | LYS  | N-CA-C | -6.80 | 104.93      | 113.23   |
| 2   | QB    | 192 | LYS  | N-CA-C | -6.80 | 104.93      | 113.23   |
| 2   | QE    | 192 | LYS  | N-CA-C | -6.80 | 104.93      | 113.23   |
| 2   | IF    | 192 | LYS  | N-CA-C | -6.80 | 104.93      | 113.23   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | YD    | 192 | LYS  | N-CA-C | -6.80 | 104.93      | 113.23   |
| 2   | J     | 192 | LYS  | N-CA-C | -6.80 | 104.94      | 113.23   |
| 2   | YA    | 192 | LYS  | N-CA-C | -6.80 | 104.94      | 113.23   |
| 2   | OC    | 192 | LYS  | N-CA-C | -6.80 | 104.94      | 113.23   |
| 2   | T     | 192 | LYS  | N-CA-C | -6.79 | 104.94      | 113.23   |
| 2   | SD    | 192 | LYS  | N-CA-C | -6.79 | 104.94      | 113.23   |
| 2   | AA    | 192 | LYS  | N-CA-C | -6.79 | 104.95      | 113.23   |
| 2   | B     | 192 | LYS  | N-CA-C | -6.78 | 104.96      | 113.23   |
| 2   | GD    | 192 | LYS  | N-CA-C | -6.78 | 104.96      | 113.23   |
| 2   | WE    | 192 | LYS  | N-CA-C | -6.78 | 104.96      | 113.23   |
| 2   | GG    | 192 | LYS  | N-CA-C | -6.78 | 104.96      | 113.23   |
| 2   | CC    | 192 | LYS  | N-CA-C | -6.77 | 104.97      | 113.23   |
| 2   | OF    | 192 | LYS  | N-CA-C | -6.77 | 104.97      | 113.23   |
| 2   | SA    | 192 | LYS  | N-CA-C | -6.77 | 104.97      | 113.23   |
| 2   | GA    | 192 | LYS  | N-CA-C | -6.76 | 104.98      | 113.23   |
| 2   | MA    | 192 | LYS  | N-CA-C | -6.76 | 104.98      | 113.23   |
| 2   | MG    | 192 | LYS  | N-CA-C | -6.76 | 104.98      | 113.23   |
| 2   | EB    | 192 | LYS  | N-CA-C | -6.76 | 104.98      | 113.23   |
| 2   | WB    | 192 | LYS  | N-CA-C | -6.75 | 104.99      | 113.23   |
| 2   | UF    | 192 | LYS  | N-CA-C | -6.75 | 104.99      | 113.23   |
| 2   | AG    | 192 | LYS  | N-CA-C | -6.75 | 105.00      | 113.23   |
| 2   | EE    | 192 | LYS  | N-CA-C | -6.74 | 105.00      | 113.23   |
| 2   | SA    | 207 | LYS  | O-C-N  | -5.87 | 116.10      | 122.79   |
| 2   | UF    | 207 | LYS  | O-C-N  | -5.84 | 116.13      | 122.79   |
| 2   | IF    | 207 | LYS  | O-C-N  | -5.84 | 116.13      | 122.79   |
| 2   | OC    | 207 | LYS  | O-C-N  | -5.83 | 116.14      | 122.79   |
| 2   | QE    | 207 | LYS  | O-C-N  | -5.83 | 116.14      | 122.79   |
| 2   | CF    | 207 | LYS  | O-C-N  | -5.83 | 116.14      | 122.79   |
| 2   | GA    | 207 | LYS  | O-C-N  | -5.83 | 116.15      | 122.79   |
| 2   | WB    | 207 | LYS  | O-C-N  | -5.83 | 116.15      | 122.79   |
| 2   | CC    | 207 | LYS  | O-C-N  | -5.82 | 116.16      | 122.79   |
| 2   | AG    | 207 | LYS  | O-C-N  | -5.82 | 116.16      | 122.79   |
| 2   | YD    | 207 | LYS  | O-C-N  | -5.81 | 116.16      | 122.79   |
| 2   | OF    | 207 | LYS  | O-C-N  | -5.81 | 116.16      | 122.79   |
| 2   | B     | 207 | LYS  | O-C-N  | -5.81 | 116.17      | 122.79   |
| 2   | AA    | 207 | LYS  | O-C-N  | -5.81 | 116.17      | 122.79   |
| 2   | J     | 207 | LYS  | O-C-N  | -5.80 | 116.18      | 122.79   |
| 2   | MA    | 207 | LYS  | O-C-N  | -5.80 | 116.18      | 122.79   |
| 2   | KE    | 207 | LYS  | O-C-N  | -5.80 | 116.18      | 122.79   |
| 2   | QB    | 207 | LYS  | O-C-N  | -5.79 | 116.19      | 122.79   |
| 2   | T     | 207 | LYS  | O-C-N  | -5.79 | 116.19      | 122.79   |
| 2   | YA    | 207 | LYS  | O-C-N  | -5.79 | 116.19      | 122.79   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | WE    | 207 | LYS  | O-C-N  | -5.79 | 116.19      | 122.79   |
| 2   | EB    | 207 | LYS  | O-C-N  | -5.78 | 116.20      | 122.79   |
| 2   | KB    | 207 | LYS  | O-C-N  | -5.78 | 116.21      | 122.79   |
| 2   | MD    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | EE    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | SG    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | G     | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | IC    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | AD    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | GG    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | SD    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | UC    | 207 | LYS  | O-C-N  | -5.77 | 116.21      | 122.79   |
| 2   | MG    | 207 | LYS  | O-C-N  | -5.76 | 116.23      | 122.79   |
| 2   | SA    | 190 | ARG  | CA-C-N | -5.74 | 114.66      | 123.04   |
| 2   | SA    | 190 | ARG  | C-N-CA | -5.74 | 114.66      | 123.04   |
| 2   | YA    | 190 | ARG  | CA-C-N | -5.74 | 114.67      | 123.04   |
| 2   | YA    | 190 | ARG  | C-N-CA | -5.74 | 114.67      | 123.04   |
| 2   | QB    | 190 | ARG  | CA-C-N | -5.73 | 114.67      | 123.04   |
| 2   | QB    | 190 | ARG  | C-N-CA | -5.73 | 114.67      | 123.04   |
| 2   | WB    | 190 | ARG  | CA-C-N | -5.73 | 114.67      | 123.04   |
| 2   | WB    | 190 | ARG  | C-N-CA | -5.73 | 114.67      | 123.04   |
| 2   | GD    | 190 | ARG  | CA-C-N | -5.73 | 114.67      | 123.04   |
| 2   | GD    | 190 | ARG  | C-N-CA | -5.73 | 114.67      | 123.04   |
| 2   | IF    | 190 | ARG  | CA-C-N | -5.73 | 114.68      | 123.04   |
| 2   | IF    | 190 | ARG  | C-N-CA | -5.73 | 114.68      | 123.04   |
| 2   | J     | 190 | ARG  | CA-C-N | -5.72 | 114.69      | 123.04   |
| 2   | J     | 190 | ARG  | C-N-CA | -5.72 | 114.69      | 123.04   |
| 2   | AD    | 190 | ARG  | CA-C-N | -5.72 | 114.69      | 123.04   |
| 2   | AD    | 190 | ARG  | C-N-CA | -5.72 | 114.69      | 123.04   |
| 2   | MG    | 190 | ARG  | CA-C-N | -5.72 | 114.69      | 123.04   |
| 2   | MG    | 190 | ARG  | C-N-CA | -5.72 | 114.69      | 123.04   |
| 2   | QE    | 190 | ARG  | CA-C-N | -5.72 | 114.69      | 123.04   |
| 2   | QE    | 190 | ARG  | C-N-CA | -5.72 | 114.69      | 123.04   |
| 2   | AA    | 190 | ARG  | CA-C-N | -5.72 | 114.69      | 123.04   |
| 2   | AA    | 190 | ARG  | C-N-CA | -5.72 | 114.69      | 123.04   |
| 2   | GD    | 207 | LYS  | O-C-N  | -5.72 | 116.27      | 122.79   |
| 2   | YD    | 190 | ARG  | CA-C-N | -5.72 | 114.69      | 123.04   |
| 2   | YD    | 190 | ARG  | C-N-CA | -5.72 | 114.69      | 123.04   |
| 2   | SG    | 190 | ARG  | CA-C-N | -5.72 | 114.69      | 123.04   |
| 2   | SG    | 190 | ARG  | C-N-CA | -5.72 | 114.69      | 123.04   |
| 2   | SD    | 190 | ARG  | CA-C-N | -5.71 | 114.70      | 123.04   |
| 2   | SD    | 190 | ARG  | C-N-CA | -5.71 | 114.70      | 123.04   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | WE    | 190 | ARG  | CA-C-N | -5.71 | 114.70      | 123.04   |
| 2   | WE    | 190 | ARG  | C-N-CA | -5.71 | 114.70      | 123.04   |
| 2   | B     | 190 | ARG  | CA-C-N | -5.71 | 114.70      | 123.04   |
| 2   | B     | 190 | ARG  | C-N-CA | -5.71 | 114.70      | 123.04   |
| 2   | CF    | 190 | ARG  | CA-C-N | -5.71 | 114.71      | 123.04   |
| 2   | CF    | 190 | ARG  | C-N-CA | -5.71 | 114.71      | 123.04   |
| 2   | UF    | 190 | ARG  | CA-C-N | -5.71 | 114.71      | 123.04   |
| 2   | UF    | 190 | ARG  | C-N-CA | -5.71 | 114.71      | 123.04   |
| 2   | EE    | 190 | ARG  | CA-C-N | -5.71 | 114.71      | 123.04   |
| 2   | EE    | 190 | ARG  | C-N-CA | -5.71 | 114.71      | 123.04   |
| 2   | KE    | 190 | ARG  | CA-C-N | -5.70 | 114.71      | 123.04   |
| 2   | KE    | 190 | ARG  | C-N-CA | -5.70 | 114.71      | 123.04   |
| 2   | OF    | 190 | ARG  | CA-C-N | -5.70 | 114.71      | 123.04   |
| 2   | OF    | 190 | ARG  | C-N-CA | -5.70 | 114.71      | 123.04   |
| 2   | KB    | 190 | ARG  | CA-C-N | -5.70 | 114.72      | 123.04   |
| 2   | KB    | 190 | ARG  | C-N-CA | -5.70 | 114.72      | 123.04   |
| 2   | AG    | 190 | ARG  | CA-C-N | -5.70 | 114.72      | 123.04   |
| 2   | AG    | 190 | ARG  | C-N-CA | -5.70 | 114.72      | 123.04   |
| 2   | UC    | 190 | ARG  | CA-C-N | -5.70 | 114.72      | 123.04   |
| 2   | UC    | 190 | ARG  | C-N-CA | -5.70 | 114.72      | 123.04   |
| 2   | MD    | 190 | ARG  | CA-C-N | -5.70 | 114.72      | 123.04   |
| 2   | MD    | 190 | ARG  | C-N-CA | -5.70 | 114.72      | 123.04   |
| 2   | T     | 190 | ARG  | CA-C-N | -5.69 | 114.74      | 123.04   |
| 2   | T     | 190 | ARG  | C-N-CA | -5.69 | 114.74      | 123.04   |
| 2   | EB    | 190 | ARG  | CA-C-N | -5.69 | 114.74      | 123.04   |
| 2   | EB    | 190 | ARG  | C-N-CA | -5.69 | 114.74      | 123.04   |
| 2   | MA    | 190 | ARG  | CA-C-N | -5.68 | 114.74      | 123.04   |
| 2   | MA    | 190 | ARG  | C-N-CA | -5.68 | 114.74      | 123.04   |
| 2   | OC    | 190 | ARG  | CA-C-N | -5.68 | 114.75      | 123.04   |
| 2   | OC    | 190 | ARG  | C-N-CA | -5.68 | 114.75      | 123.04   |
| 2   | GA    | 190 | ARG  | CA-C-N | -5.68 | 114.75      | 123.04   |
| 2   | GA    | 190 | ARG  | C-N-CA | -5.68 | 114.75      | 123.04   |
| 2   | G     | 190 | ARG  | CA-C-N | -5.68 | 114.75      | 123.04   |
| 2   | G     | 190 | ARG  | C-N-CA | -5.68 | 114.75      | 123.04   |
| 2   | CC    | 190 | ARG  | CA-C-N | -5.67 | 114.76      | 123.04   |
| 2   | CC    | 190 | ARG  | C-N-CA | -5.67 | 114.76      | 123.04   |
| 2   | IC    | 190 | ARG  | CA-C-N | -5.67 | 114.76      | 123.04   |
| 2   | IC    | 190 | ARG  | C-N-CA | -5.67 | 114.76      | 123.04   |
| 2   | GG    | 190 | ARG  | CA-C-N | -5.67 | 114.76      | 123.04   |
| 2   | GG    | 190 | ARG  | C-N-CA | -5.67 | 114.76      | 123.04   |

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     | 234   | 0        | 102      | 1       | 0            |
| 1   | BC    | 234   | 0        | 102      | 1       | 0            |
| 1   | BF    | 234   | 0        | 102      | 1       | 0            |
| 1   | DB    | 234   | 0        | 102      | 1       | 0            |
| 1   | DE    | 234   | 0        | 102      | 1       | 0            |
| 1   | F     | 234   | 0        | 102      | 1       | 0            |
| 1   | FA    | 234   | 0        | 102      | 1       | 0            |
| 1   | FD    | 234   | 0        | 102      | 1       | 0            |
| 1   | FG    | 234   | 0        | 102      | 1       | 0            |
| 1   | HC    | 234   | 0        | 102      | 1       | 0            |
| 1   | HF    | 234   | 0        | 102      | 1       | 0            |
| 1   | I     | 234   | 0        | 102      | 1       | 0            |
| 1   | JB    | 234   | 0        | 102      | 1       | 0            |
| 1   | JE    | 234   | 0        | 102      | 1       | 0            |
| 1   | LA    | 234   | 0        | 102      | 1       | 0            |
| 1   | LD    | 234   | 0        | 102      | 1       | 0            |
| 1   | LG    | 234   | 0        | 102      | 1       | 0            |
| 1   | NC    | 234   | 0        | 102      | 1       | 0            |
| 1   | NF    | 234   | 0        | 102      | 1       | 0            |
| 1   | PB    | 234   | 0        | 102      | 1       | 0            |
| 1   | PE    | 234   | 0        | 102      | 1       | 0            |
| 1   | RA    | 234   | 0        | 102      | 1       | 0            |
| 1   | RD    | 234   | 0        | 102      | 1       | 0            |
| 1   | RG    | 234   | 0        | 102      | 1       | 0            |
| 1   | S     | 234   | 0        | 102      | 1       | 0            |
| 1   | TC    | 234   | 0        | 102      | 1       | 0            |
| 1   | TF    | 234   | 0        | 102      | 1       | 0            |
| 1   | VB    | 234   | 0        | 102      | 1       | 0            |
| 1   | VE    | 234   | 0        | 102      | 1       | 0            |
| 1   | XA    | 234   | 0        | 102      | 1       | 0            |
| 1   | XD    | 234   | 0        | 102      | 1       | 0            |
| 1   | Z     | 234   | 0        | 102      | 1       | 0            |
| 1   | ZC    | 234   | 0        | 102      | 1       | 0            |
| 1   | ZF    | 234   | 0        | 102      | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | AA    | 1579  | 0        | 738      | 50      | 0            |
| 2   | AD    | 1579  | 0        | 738      | 49      | 0            |
| 2   | AG    | 1579  | 0        | 738      | 49      | 0            |
| 2   | B     | 1579  | 0        | 738      | 49      | 0            |
| 2   | CC    | 1579  | 0        | 738      | 49      | 0            |
| 2   | CF    | 1579  | 0        | 738      | 48      | 0            |
| 2   | EB    | 1579  | 0        | 738      | 50      | 0            |
| 2   | EE    | 1579  | 0        | 738      | 48      | 0            |
| 2   | G     | 1579  | 0        | 738      | 49      | 0            |
| 2   | GA    | 1579  | 0        | 738      | 51      | 0            |
| 2   | GD    | 1579  | 0        | 738      | 51      | 0            |
| 2   | GG    | 1579  | 0        | 738      | 48      | 0            |
| 2   | IC    | 1579  | 0        | 738      | 50      | 0            |
| 2   | IF    | 1579  | 0        | 738      | 49      | 0            |
| 2   | J     | 1579  | 0        | 738      | 49      | 0            |
| 2   | KB    | 1579  | 0        | 738      | 50      | 0            |
| 2   | KE    | 1579  | 0        | 738      | 51      | 0            |
| 2   | MA    | 1579  | 0        | 738      | 48      | 0            |
| 2   | MD    | 1579  | 0        | 738      | 49      | 0            |
| 2   | MG    | 1579  | 0        | 738      | 47      | 0            |
| 2   | OC    | 1579  | 0        | 738      | 52      | 0            |
| 2   | OF    | 1579  | 0        | 738      | 49      | 0            |
| 2   | QB    | 1579  | 0        | 738      | 49      | 0            |
| 2   | QE    | 1579  | 0        | 738      | 51      | 0            |
| 2   | SA    | 1579  | 0        | 738      | 47      | 0            |
| 2   | SD    | 1579  | 0        | 738      | 48      | 0            |
| 2   | SG    | 1579  | 0        | 738      | 49      | 0            |
| 2   | T     | 1579  | 0        | 738      | 49      | 0            |
| 2   | UC    | 1579  | 0        | 738      | 50      | 0            |
| 2   | UF    | 1579  | 0        | 738      | 49      | 0            |
| 2   | WB    | 1579  | 0        | 738      | 48      | 0            |
| 2   | WE    | 1579  | 0        | 738      | 49      | 0            |
| 2   | YA    | 1579  | 0        | 738      | 49      | 0            |
| 2   | YD    | 1579  | 0        | 738      | 48      | 0            |
| 3   | BA    | 1420  | 0        | 604      | 16      | 0            |
| 3   | BD    | 1420  | 0        | 604      | 17      | 0            |
| 3   | BG    | 1420  | 0        | 604      | 16      | 0            |
| 3   | C     | 1420  | 0        | 604      | 16      | 0            |
| 3   | DC    | 1420  | 0        | 604      | 17      | 0            |
| 3   | DF    | 1420  | 0        | 604      | 16      | 0            |
| 3   | FB    | 1420  | 0        | 604      | 17      | 0            |
| 3   | FE    | 1420  | 0        | 604      | 16      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | HA    | 1420  | 0        | 604      | 16      | 0            |
| 3   | HD    | 1420  | 0        | 604      | 16      | 0            |
| 3   | HG    | 1420  | 0        | 604      | 16      | 0            |
| 3   | JC    | 1420  | 0        | 604      | 16      | 0            |
| 3   | JF    | 1420  | 0        | 604      | 16      | 0            |
| 3   | K     | 1420  | 0        | 604      | 16      | 0            |
| 3   | LB    | 1420  | 0        | 604      | 17      | 0            |
| 3   | LE    | 1420  | 0        | 604      | 17      | 0            |
| 3   | M     | 1420  | 0        | 604      | 16      | 0            |
| 3   | NA    | 1420  | 0        | 604      | 16      | 0            |
| 3   | ND    | 1420  | 0        | 604      | 16      | 0            |
| 3   | NG    | 1420  | 0        | 604      | 16      | 0            |
| 3   | PC    | 1420  | 0        | 604      | 16      | 0            |
| 3   | PF    | 1420  | 0        | 604      | 16      | 0            |
| 3   | RB    | 1420  | 0        | 604      | 16      | 0            |
| 3   | RE    | 1420  | 0        | 604      | 16      | 0            |
| 3   | TA    | 1420  | 0        | 604      | 16      | 0            |
| 3   | TD    | 1420  | 0        | 604      | 16      | 0            |
| 3   | TG    | 1420  | 0        | 604      | 16      | 0            |
| 3   | V     | 1420  | 0        | 604      | 16      | 0            |
| 3   | VC    | 1420  | 0        | 604      | 17      | 0            |
| 3   | VF    | 1420  | 0        | 604      | 16      | 0            |
| 3   | XB    | 1420  | 0        | 604      | 16      | 0            |
| 3   | XE    | 1420  | 0        | 604      | 16      | 0            |
| 3   | ZA    | 1420  | 0        | 604      | 17      | 0            |
| 3   | ZD    | 1420  | 0        | 604      | 16      | 0            |
| 4   | AB    | 456   | 0        | 206      | 5       | 0            |
| 4   | AC    | 399   | 0        | 177      | 9       | 0            |
| 4   | AE    | 456   | 0        | 206      | 6       | 0            |
| 4   | AF    | 399   | 0        | 177      | 9       | 0            |
| 4   | BB    | 409   | 0        | 181      | 6       | 0            |
| 4   | BE    | 409   | 0        | 181      | 7       | 0            |
| 4   | CA    | 456   | 0        | 206      | 6       | 0            |
| 4   | CB    | 399   | 0        | 177      | 10      | 0            |
| 4   | CD    | 456   | 0        | 206      | 6       | 0            |
| 4   | CE    | 399   | 0        | 177      | 9       | 0            |
| 4   | CG    | 456   | 0        | 206      | 6       | 0            |
| 4   | D     | 456   | 0        | 206      | 6       | 0            |
| 4   | DA    | 409   | 0        | 181      | 6       | 0            |
| 4   | DD    | 409   | 0        | 181      | 7       | 0            |
| 4   | DG    | 409   | 0        | 181      | 6       | 0            |
| 4   | E     | 409   | 0        | 181      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | EA    | 399   | 0        | 177      | 9       | 0            |
| 4   | EC    | 456   | 0        | 206      | 6       | 0            |
| 4   | ED    | 399   | 0        | 177      | 10      | 0            |
| 4   | EF    | 456   | 0        | 206      | 6       | 0            |
| 4   | EG    | 399   | 0        | 177      | 10      | 0            |
| 4   | FC    | 409   | 0        | 181      | 6       | 0            |
| 4   | FF    | 409   | 0        | 181      | 7       | 0            |
| 4   | GB    | 456   | 0        | 206      | 5       | 0            |
| 4   | GC    | 399   | 0        | 177      | 9       | 0            |
| 4   | GE    | 456   | 0        | 206      | 6       | 0            |
| 4   | GF    | 399   | 0        | 177      | 9       | 0            |
| 4   | H     | 399   | 0        | 177      | 10      | 0            |
| 4   | HB    | 409   | 0        | 181      | 6       | 0            |
| 4   | HE    | 409   | 0        | 181      | 7       | 0            |
| 4   | IA    | 456   | 0        | 206      | 5       | 0            |
| 4   | IB    | 399   | 0        | 177      | 10      | 0            |
| 4   | ID    | 456   | 0        | 206      | 6       | 0            |
| 4   | IE    | 399   | 0        | 177      | 9       | 0            |
| 4   | IG    | 456   | 0        | 206      | 6       | 0            |
| 4   | JA    | 409   | 0        | 181      | 6       | 0            |
| 4   | JD    | 409   | 0        | 181      | 6       | 0            |
| 4   | JG    | 409   | 0        | 181      | 6       | 0            |
| 4   | KA    | 399   | 0        | 177      | 10      | 0            |
| 4   | KC    | 456   | 0        | 206      | 6       | 0            |
| 4   | KD    | 399   | 0        | 177      | 10      | 0            |
| 4   | KF    | 456   | 0        | 206      | 6       | 0            |
| 4   | KG    | 399   | 0        | 177      | 10      | 0            |
| 4   | L     | 456   | 0        | 206      | 6       | 0            |
| 4   | LC    | 409   | 0        | 181      | 6       | 0            |
| 4   | LF    | 409   | 0        | 181      | 7       | 0            |
| 4   | MB    | 456   | 0        | 206      | 5       | 0            |
| 4   | MC    | 399   | 0        | 177      | 9       | 0            |
| 4   | ME    | 456   | 0        | 206      | 6       | 0            |
| 4   | MF    | 399   | 0        | 177      | 9       | 0            |
| 4   | N     | 456   | 0        | 206      | 6       | 0            |
| 4   | NB    | 409   | 0        | 181      | 6       | 0            |
| 4   | NE    | 409   | 0        | 181      | 7       | 0            |
| 4   | O     | 409   | 0        | 181      | 7       | 0            |
| 4   | OA    | 456   | 0        | 206      | 6       | 0            |
| 4   | OB    | 399   | 0        | 177      | 10      | 0            |
| 4   | OD    | 456   | 0        | 206      | 7       | 0            |
| 4   | OE    | 399   | 0        | 177      | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | OG    | 456   | 0        | 206      | 6       | 0            |
| 4   | P     | 409   | 0        | 181      | 6       | 0            |
| 4   | PA    | 409   | 0        | 181      | 7       | 0            |
| 4   | PD    | 409   | 0        | 181      | 6       | 0            |
| 4   | PG    | 409   | 0        | 181      | 6       | 0            |
| 4   | Q     | 399   | 0        | 177      | 10      | 0            |
| 4   | QA    | 399   | 0        | 177      | 10      | 0            |
| 4   | QC    | 456   | 0        | 206      | 6       | 0            |
| 4   | QD    | 399   | 0        | 177      | 10      | 0            |
| 4   | QF    | 456   | 0        | 206      | 6       | 0            |
| 4   | QG    | 399   | 0        | 177      | 10      | 0            |
| 4   | R     | 399   | 0        | 177      | 9       | 0            |
| 4   | RC    | 409   | 0        | 181      | 7       | 0            |
| 4   | RF    | 409   | 0        | 181      | 7       | 0            |
| 4   | SB    | 456   | 0        | 206      | 6       | 0            |
| 4   | SC    | 399   | 0        | 177      | 9       | 0            |
| 4   | SE    | 456   | 0        | 206      | 6       | 0            |
| 4   | SF    | 399   | 0        | 177      | 9       | 0            |
| 4   | TB    | 409   | 0        | 181      | 7       | 0            |
| 4   | TE    | 409   | 0        | 181      | 6       | 0            |
| 4   | UA    | 456   | 0        | 206      | 5       | 0            |
| 4   | UB    | 399   | 0        | 177      | 10      | 0            |
| 4   | UD    | 456   | 0        | 206      | 7       | 0            |
| 4   | UE    | 399   | 0        | 177      | 10      | 0            |
| 4   | UG    | 456   | 0        | 206      | 6       | 0            |
| 4   | VA    | 409   | 0        | 181      | 6       | 0            |
| 4   | VD    | 409   | 0        | 181      | 7       | 0            |
| 4   | VG    | 409   | 0        | 181      | 7       | 0            |
| 4   | W     | 456   | 0        | 206      | 6       | 0            |
| 4   | WA    | 399   | 0        | 177      | 10      | 0            |
| 4   | WC    | 456   | 0        | 206      | 6       | 0            |
| 4   | WD    | 399   | 0        | 177      | 10      | 0            |
| 4   | WF    | 456   | 0        | 206      | 6       | 0            |
| 4   | WG    | 399   | 0        | 177      | 10      | 0            |
| 4   | X     | 409   | 0        | 181      | 7       | 0            |
| 4   | XC    | 409   | 0        | 181      | 7       | 0            |
| 4   | XF    | 409   | 0        | 181      | 6       | 0            |
| 4   | Y     | 399   | 0        | 177      | 9       | 0            |
| 4   | YB    | 456   | 0        | 206      | 6       | 0            |
| 4   | YC    | 399   | 0        | 177      | 9       | 0            |
| 4   | YE    | 456   | 0        | 206      | 6       | 0            |
| 4   | YF    | 399   | 0        | 177      | 10      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 4   | ZB    | 409    | 0        | 181      | 7       | 0            |
| 4   | ZE    | 409    | 0        | 181      | 6       | 0            |
| All | All   | 152898 | 0        | 68272    | 2191    | 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 10.

All (2191) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:KE:77:LEU:CB  | 2:QE:42:ALA:HA  | 1.55                     | 1.35              |
| 2:MA:200:ALA:CB | 2:MA:232:GLU:CB | 2.05                     | 1.35              |
| 2:QB:200:ALA:CB | 2:QB:232:GLU:CB | 2.05                     | 1.35              |
| 2:WB:200:ALA:CB | 2:WB:232:GLU:CB | 2.05                     | 1.35              |
| 2:GD:200:ALA:CB | 2:GD:232:GLU:CB | 2.05                     | 1.35              |
| 2:QE:200:ALA:CB | 2:QE:232:GLU:CB | 2.05                     | 1.35              |
| 2:SA:200:ALA:CB | 2:SA:232:GLU:CB | 2.05                     | 1.35              |
| 2:AD:200:ALA:CB | 2:AD:232:GLU:CB | 2.05                     | 1.35              |
| 2:MD:200:ALA:CB | 2:MD:232:GLU:CB | 2.05                     | 1.35              |
| 2:KE:200:ALA:CB | 2:KE:232:GLU:CB | 2.05                     | 1.35              |
| 2:GA:200:ALA:CB | 2:GA:232:GLU:CB | 2.05                     | 1.34              |
| 2:CC:200:ALA:CB | 2:CC:232:GLU:CB | 2.05                     | 1.34              |
| 2:KB:200:ALA:CB | 2:KB:232:GLU:CB | 2.05                     | 1.34              |
| 2:UC:200:ALA:CB | 2:UC:232:GLU:CB | 2.05                     | 1.34              |
| 2:EE:200:ALA:CB | 2:EE:232:GLU:CB | 2.05                     | 1.34              |
| 2:WE:200:ALA:CB | 2:WE:232:GLU:CB | 2.05                     | 1.34              |
| 2:GA:77:LEU:CB  | 2:MA:42:ALA:HA  | 1.58                     | 1.34              |
| 2:SD:200:ALA:CB | 2:SD:232:GLU:CB | 2.05                     | 1.34              |
| 2:YA:200:ALA:CB | 2:YA:232:GLU:CB | 2.05                     | 1.34              |
| 2:OC:77:LEU:CB  | 2:UC:42:ALA:HA  | 1.55                     | 1.34              |
| 2:G:200:ALA:CB  | 2:G:232:GLU:CB  | 2.05                     | 1.33              |
| 2:B:200:ALA:CB  | 2:B:232:GLU:CB  | 2.05                     | 1.33              |
| 2:AA:200:ALA:CB | 2:AA:232:GLU:CB | 2.05                     | 1.33              |
| 2:IC:200:ALA:CB | 2:IC:232:GLU:CB | 2.05                     | 1.33              |
| 2:UF:200:ALA:CB | 2:UF:232:GLU:CB | 2.05                     | 1.33              |
| 2:OF:200:ALA:CB | 2:OF:232:GLU:CB | 2.05                     | 1.33              |
| 2:J:200:ALA:CB  | 2:J:232:GLU:CB  | 2.05                     | 1.33              |
| 2:AG:200:ALA:CB | 2:AG:232:GLU:CB | 2.05                     | 1.33              |
| 2:EB:200:ALA:CB | 2:EB:232:GLU:CB | 2.05                     | 1.33              |
| 2:YD:200:ALA:CB | 2:YD:232:GLU:CB | 2.05                     | 1.33              |
| 2:OC:200:ALA:CB | 2:OC:232:GLU:CB | 2.05                     | 1.32              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:AD:77:LEU:CB  | 2:GD:42:ALA:HA  | 1.58                     | 1.32              |
| 2:CF:200:ALA:CB | 2:CF:232:GLU:CB | 2.05                     | 1.32              |
| 2:SG:200:ALA:CB | 2:SG:232:GLU:CB | 2.05                     | 1.32              |
| 2:G:42:ALA:HA   | 2:SG:77:LEU:CB  | 1.60                     | 1.32              |
| 2:IF:200:ALA:CB | 2:IF:232:GLU:CB | 2.05                     | 1.32              |
| 2:GG:200:ALA:CB | 2:GG:232:GLU:CB | 2.05                     | 1.32              |
| 2:T:200:ALA:CB  | 2:T:232:GLU:CB  | 2.05                     | 1.32              |
| 2:T:77:LEU:CB   | 2:AA:42:ALA:HA  | 1.60                     | 1.31              |
| 2:MG:200:ALA:CB | 2:MG:232:GLU:CB | 2.05                     | 1.31              |
| 2:AG:77:LEU:CB  | 2:GG:42:ALA:HA  | 1.60                     | 1.31              |
| 2:KB:77:LEU:CB  | 2:QB:42:ALA:HA  | 1.60                     | 1.31              |
| 2:WB:77:LEU:CB  | 2:CC:42:ALA:HA  | 1.60                     | 1.31              |
| 2:IF:77:LEU:CB  | 2:OF:42:ALA:HA  | 1.62                     | 1.30              |
| 2:YA:77:LEU:CB  | 2:EB:42:ALA:HA  | 1.61                     | 1.29              |
| 2:OF:77:LEU:CB  | 2:UF:42:ALA:HA  | 1.60                     | 1.29              |
| 2:IC:77:LEU:CB  | 2:OC:42:ALA:HA  | 1.60                     | 1.29              |
| 2:QE:77:LEU:CB  | 2:WE:42:ALA:HA  | 1.62                     | 1.29              |
| 2:J:77:LEU:CB   | 2:T:42:ALA:HA   | 1.61                     | 1.29              |
| 2:AA:77:LEU:CB  | 2:GA:42:ALA:HA  | 1.63                     | 1.29              |
| 2:EB:77:LEU:CB  | 2:KB:42:ALA:HA  | 1.61                     | 1.29              |
| 2:GG:77:LEU:CB  | 2:MG:42:ALA:HA  | 1.64                     | 1.28              |
| 2:CF:77:LEU:CB  | 2:IF:42:ALA:HA  | 1.64                     | 1.28              |
| 2:KB:74:ASN:N   | 2:QB:42:ALA:O   | 1.64                     | 1.28              |
| 2:B:77:LEU:CB   | 2:J:42:ALA:HA   | 1.62                     | 1.28              |
| 2:SA:77:LEU:CB  | 2:YA:42:ALA:HA  | 1.63                     | 1.27              |
| 2:OC:74:ASN:N   | 2:UC:42:ALA:O   | 1.65                     | 1.27              |
| 2:GD:77:LEU:CB  | 2:MD:42:ALA:HA  | 1.63                     | 1.27              |
| 2:UF:77:LEU:CB  | 2:AG:42:ALA:HA  | 1.64                     | 1.26              |
| 2:SD:77:LEU:CB  | 2:YD:42:ALA:HA  | 1.65                     | 1.26              |
| 2:WE:77:LEU:CB  | 2:CF:42:ALA:HA  | 1.66                     | 1.26              |
| 2:YD:77:LEU:CB  | 2:EE:42:ALA:HA  | 1.63                     | 1.25              |
| 2:G:77:LEU:CB   | 2:B:42:ALA:HA   | 1.66                     | 1.25              |
| 2:MG:77:LEU:CB  | 2:SG:42:ALA:HA  | 1.67                     | 1.25              |
| 2:CC:77:LEU:CB  | 2:IC:42:ALA:HA  | 1.66                     | 1.24              |
| 2:MD:77:LEU:CB  | 2:SD:42:ALA:HA  | 1.66                     | 1.24              |
| 2:OF:74:ASN:N   | 2:UF:42:ALA:O   | 1.69                     | 1.24              |
| 2:GA:74:ASN:N   | 2:MA:42:ALA:O   | 1.69                     | 1.23              |
| 2:QB:77:LEU:CB  | 2:WB:42:ALA:HA  | 1.67                     | 1.23              |
| 2:EE:77:LEU:CB  | 2:KE:42:ALA:HA  | 1.66                     | 1.23              |
| 2:KE:74:ASN:N   | 2:QE:42:ALA:O   | 1.70                     | 1.23              |
| 2:AD:74:ASN:N   | 2:GD:42:ALA:O   | 1.69                     | 1.22              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:MA:77:LEU:CB   | 2:SA:42:ALA:HA  | 1.69                     | 1.22              |
| 2:T:74:ASN:N     | 2:AA:42:ALA:O   | 1.70                     | 1.22              |
| 2:AG:74:ASN:N    | 2:GG:42:ALA:O   | 1.70                     | 1.22              |
| 2:UC:77:LEU:CB   | 2:AD:42:ALA:HA  | 1.68                     | 1.22              |
| 2:QE:74:ASN:N    | 2:WE:42:ALA:O   | 1.71                     | 1.21              |
| 2:MA:74:ASN:N    | 2:SA:42:ALA:O   | 1.71                     | 1.21              |
| 2:YD:74:ASN:N    | 2:EE:42:ALA:O   | 1.70                     | 1.21              |
| 2:EB:74:ASN:N    | 2:KB:42:ALA:O   | 1.72                     | 1.21              |
| 2:GG:74:ASN:N    | 2:MG:42:ALA:O   | 1.70                     | 1.21              |
| 2:WB:74:ASN:N    | 2:CC:42:ALA:O   | 1.73                     | 1.21              |
| 2:WE:74:ASN:N    | 2:CF:42:ALA:O   | 1.70                     | 1.21              |
| 2:G:42:ALA:O     | 2:SG:74:ASN:N   | 1.72                     | 1.20              |
| 2:CC:200:ALA:HB2 | 2:CC:232:GLU:CB | 1.71                     | 1.20              |
| 2:CF:74:ASN:N    | 2:IF:42:ALA:O   | 1.73                     | 1.19              |
| 2:UF:74:ASN:N    | 2:AG:42:ALA:O   | 1.72                     | 1.19              |
| 2:IC:200:ALA:HB2 | 2:IC:232:GLU:CB | 1.71                     | 1.19              |
| 2:SA:74:ASN:N    | 2:YA:42:ALA:O   | 1.74                     | 1.19              |
| 2:MD:74:ASN:N    | 2:SD:42:ALA:O   | 1.71                     | 1.19              |
| 2:B:74:ASN:N     | 2:J:42:ALA:O    | 1.72                     | 1.19              |
| 2:GD:74:ASN:N    | 2:MD:42:ALA:O   | 1.72                     | 1.18              |
| 2:WB:200:ALA:HB2 | 2:WB:232:GLU:CB | 1.71                     | 1.18              |
| 2:J:74:ASN:N     | 2:T:42:ALA:O    | 1.74                     | 1.18              |
| 2:AA:74:ASN:N    | 2:GA:42:ALA:O   | 1.75                     | 1.18              |
| 2:OC:200:ALA:HB2 | 2:OC:232:GLU:CB | 1.71                     | 1.17              |
| 2:IC:74:ASN:N    | 2:OC:42:ALA:O   | 1.76                     | 1.17              |
| 2:YA:74:ASN:N    | 2:EB:42:ALA:O   | 1.77                     | 1.17              |
| 2:CC:74:ASN:N    | 2:IC:42:ALA:O   | 1.75                     | 1.17              |
| 2:G:74:ASN:N     | 2:B:42:ALA:O    | 1.73                     | 1.16              |
| 2:SD:74:ASN:N    | 2:YD:42:ALA:O   | 1.75                     | 1.16              |
| 2:UC:74:ASN:N    | 2:AD:42:ALA:O   | 1.74                     | 1.16              |
| 2:QB:200:ALA:HB2 | 2:QB:232:GLU:CB | 1.71                     | 1.16              |
| 2:GD:200:ALA:HB2 | 2:GD:232:GLU:CB | 1.71                     | 1.16              |
| 2:IF:74:ASN:N    | 2:OF:42:ALA:O   | 1.78                     | 1.16              |
| 2:EE:74:ASN:N    | 2:KE:42:ALA:O   | 1.77                     | 1.15              |
| 2:QB:74:ASN:N    | 2:WB:42:ALA:O   | 1.77                     | 1.15              |
| 2:UC:200:ALA:HB2 | 2:UC:232:GLU:CB | 1.70                     | 1.15              |
| 2:AD:200:ALA:HB2 | 2:AD:232:GLU:CB | 1.71                     | 1.15              |
| 2:MD:200:ALA:HB2 | 2:MD:232:GLU:CB | 1.71                     | 1.15              |
| 2:YA:200:ALA:HB2 | 2:YA:232:GLU:CB | 1.71                     | 1.15              |
| 2:KB:200:ALA:HB2 | 2:KB:232:GLU:CB | 1.71                     | 1.15              |
| 2:MG:74:ASN:N    | 2:SG:42:ALA:O   | 1.77                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:EB:200:ALA:HB2 | 2:EB:232:GLU:CB  | 1.71                     | 1.14              |
| 2:YD:200:ALA:HB2 | 2:YD:232:GLU:CB  | 1.70                     | 1.14              |
| 2:SA:200:ALA:HB2 | 2:SA:232:GLU:CB  | 1.71                     | 1.14              |
| 2:EE:200:ALA:HB2 | 2:EE:232:GLU:CB  | 1.71                     | 1.14              |
| 2:SD:200:ALA:HB2 | 2:SD:232:GLU:CB  | 1.71                     | 1.13              |
| 2:AG:200:ALA:HB2 | 2:AG:232:GLU:CB  | 1.71                     | 1.13              |
| 2:GG:200:ALA:HB2 | 2:GG:232:GLU:CB  | 1.71                     | 1.13              |
| 2:AA:200:ALA:HB2 | 2:AA:232:GLU:CB  | 1.70                     | 1.12              |
| 2:GA:200:ALA:HB2 | 2:GA:232:GLU:CB  | 1.70                     | 1.12              |
| 2:KE:200:ALA:HB2 | 2:KE:232:GLU:CB  | 1.71                     | 1.12              |
| 2:MA:200:ALA:HB2 | 2:MA:232:GLU:CB  | 1.71                     | 1.12              |
| 2:WE:200:ALA:HB2 | 2:WE:232:GLU:CB  | 1.71                     | 1.12              |
| 2:UF:200:ALA:HB2 | 2:UF:232:GLU:CB  | 1.71                     | 1.11              |
| 2:T:200:ALA:HB2  | 2:T:232:GLU:CB   | 1.71                     | 1.11              |
| 2:QE:200:ALA:HB2 | 2:QE:232:GLU:CB  | 1.71                     | 1.11              |
| 2:CF:200:ALA:HB2 | 2:CF:232:GLU:CB  | 1.71                     | 1.11              |
| 2:MG:200:ALA:HB2 | 2:MG:232:GLU:CB  | 1.71                     | 1.11              |
| 2:OC:155:HIS:CB  | 2:UC:217:ALA:CB  | 2.29                     | 1.10              |
| 2:G:200:ALA:HB2  | 2:G:232:GLU:CB   | 1.71                     | 1.10              |
| 2:B:200:ALA:HB2  | 2:B:232:GLU:CB   | 1.71                     | 1.10              |
| 2:IF:200:ALA:HB2 | 2:IF:232:GLU:CB  | 1.71                     | 1.10              |
| 2:SG:200:ALA:HB2 | 2:SG:232:GLU:CB  | 1.71                     | 1.10              |
| 2:J:200:ALA:HB2  | 2:J:232:GLU:CB   | 1.71                     | 1.09              |
| 2:OC:155:HIS:CB  | 2:UC:217:ALA:HB1 | 1.81                     | 1.09              |
| 2:OF:200:ALA:HB2 | 2:OF:232:GLU:CB  | 1.71                     | 1.09              |
| 2:KE:155:HIS:CB  | 2:QE:217:ALA:HB1 | 1.84                     | 1.08              |
| 2:KE:155:HIS:CB  | 2:QE:217:ALA:CB  | 2.30                     | 1.08              |
| 2:AD:155:HIS:CB  | 2:GD:217:ALA:CB  | 2.32                     | 1.07              |
| 2:KB:155:HIS:CB  | 2:QB:217:ALA:CB  | 2.33                     | 1.06              |
| 2:AD:155:HIS:CB  | 2:GD:217:ALA:HB1 | 1.85                     | 1.06              |
| 2:G:217:ALA:CB   | 2:SG:155:HIS:CB  | 2.34                     | 1.05              |
| 2:GA:155:HIS:CB  | 2:MA:217:ALA:HB1 | 1.86                     | 1.05              |
| 2:KB:155:HIS:CB  | 2:QB:217:ALA:HB1 | 1.85                     | 1.05              |
| 2:GA:155:HIS:CB  | 2:MA:217:ALA:CB  | 2.33                     | 1.05              |
| 2:WB:155:HIS:CB  | 2:CC:217:ALA:CB  | 2.35                     | 1.05              |
| 2:IC:200:ALA:HB1 | 2:IC:232:GLU:CB  | 1.87                     | 1.05              |
| 2:CC:200:ALA:HB1 | 2:CC:232:GLU:CB  | 1.87                     | 1.05              |
| 2:T:155:HIS:CB   | 2:AA:217:ALA:CB  | 2.34                     | 1.04              |
| 2:YA:200:ALA:HB1 | 2:YA:232:GLU:CB  | 1.87                     | 1.04              |
| 2:OF:155:HIS:CB  | 2:UF:217:ALA:HB1 | 1.87                     | 1.04              |
| 2:AG:155:HIS:CB  | 2:GG:217:ALA:CB  | 2.35                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:EB:200:ALA:HB1 | 2:EB:232:GLU:CB  | 1.87                     | 1.04              |
| 2:MD:200:ALA:HB1 | 2:MD:232:GLU:CB  | 1.87                     | 1.04              |
| 2:OF:155:HIS:CB  | 2:UF:217:ALA:CB  | 2.34                     | 1.04              |
| 2:T:155:HIS:CB   | 2:AA:217:ALA:HB1 | 1.88                     | 1.04              |
| 2:EB:155:HIS:CB  | 2:KB:217:ALA:CB  | 2.35                     | 1.04              |
| 2:GD:200:ALA:HB1 | 2:GD:232:GLU:CB  | 1.87                     | 1.04              |
| 2:IC:155:HIS:CB  | 2:OC:217:ALA:CB  | 2.36                     | 1.03              |
| 2:OC:200:ALA:HB1 | 2:OC:232:GLU:CB  | 1.87                     | 1.03              |
| 2:AG:155:HIS:CB  | 2:GG:217:ALA:HB1 | 1.88                     | 1.03              |
| 2:SA:200:ALA:HB1 | 2:SA:232:GLU:CB  | 1.87                     | 1.03              |
| 2:WB:200:ALA:HB1 | 2:WB:232:GLU:CB  | 1.87                     | 1.03              |
| 2:SD:200:ALA:HB1 | 2:SD:232:GLU:CB  | 1.87                     | 1.03              |
| 2:G:217:ALA:HB1  | 2:SG:155:HIS:CB  | 1.88                     | 1.03              |
| 2:B:155:HIS:CB   | 2:J:217:ALA:CB   | 2.36                     | 1.03              |
| 2:YA:155:HIS:CB  | 2:EB:217:ALA:CB  | 2.36                     | 1.03              |
| 2:J:155:HIS:CB   | 2:T:217:ALA:CB   | 2.36                     | 1.03              |
| 2:KB:200:ALA:HB1 | 2:KB:232:GLU:CB  | 1.87                     | 1.03              |
| 2:UF:200:ALA:HB1 | 2:UF:232:GLU:CB  | 1.87                     | 1.03              |
| 2:GD:155:HIS:CB  | 2:MD:217:ALA:CB  | 2.37                     | 1.02              |
| 2:AG:200:ALA:HB1 | 2:AG:232:GLU:CB  | 1.87                     | 1.02              |
| 2:AD:200:ALA:HB1 | 2:AD:232:GLU:CB  | 1.87                     | 1.02              |
| 2:YD:155:HIS:CB  | 2:EE:217:ALA:CB  | 2.37                     | 1.02              |
| 2:GG:155:HIS:CB  | 2:MG:217:ALA:CB  | 2.37                     | 1.02              |
| 2:EB:155:HIS:CB  | 2:KB:217:ALA:HB1 | 1.89                     | 1.02              |
| 2:QE:155:HIS:CB  | 2:WE:217:ALA:HB1 | 1.90                     | 1.02              |
| 2:QE:155:HIS:CB  | 2:WE:217:ALA:CB  | 2.36                     | 1.02              |
| 2:G:200:ALA:HB1  | 2:G:232:GLU:CB   | 1.87                     | 1.02              |
| 2:IF:155:HIS:CB  | 2:OF:217:ALA:CB  | 2.37                     | 1.02              |
| 2:B:155:HIS:CB   | 2:J:217:ALA:HB1  | 1.90                     | 1.01              |
| 2:J:155:HIS:CB   | 2:T:217:ALA:HB1  | 1.90                     | 1.01              |
| 2:T:200:ALA:HB1  | 2:T:232:GLU:CB   | 1.87                     | 1.01              |
| 2:WB:155:HIS:CB  | 2:CC:217:ALA:HB1 | 1.89                     | 1.01              |
| 2:YD:155:HIS:CB  | 2:EE:217:ALA:HB1 | 1.90                     | 1.01              |
| 2:B:200:ALA:HB1  | 2:B:232:GLU:CB   | 1.87                     | 1.01              |
| 2:AA:200:ALA:HB1 | 2:AA:232:GLU:CB  | 1.87                     | 1.01              |
| 2:SA:155:HIS:CB  | 2:YA:217:ALA:CB  | 2.38                     | 1.01              |
| 2:UC:200:ALA:HB1 | 2:UC:232:GLU:CB  | 1.87                     | 1.01              |
| 2:OF:200:ALA:HB1 | 2:OF:232:GLU:CB  | 1.87                     | 1.01              |
| 2:GG:200:ALA:HB1 | 2:GG:232:GLU:CB  | 1.87                     | 1.01              |
| 2:MA:200:ALA:HB1 | 2:MA:232:GLU:CB  | 1.87                     | 1.01              |
| 2:YD:200:ALA:HB1 | 2:YD:232:GLU:CB  | 1.87                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:WE:200:ALA:HB1 | 2:WE:232:GLU:CB  | 1.87                     | 1.01              |
| 2:UF:155:HIS:CB  | 2:AG:217:ALA:CB  | 2.38                     | 1.01              |
| 2:SG:200:ALA:HB1 | 2:SG:232:GLU:CB  | 1.87                     | 1.01              |
| 2:J:200:ALA:HB1  | 2:J:232:GLU:CB   | 1.87                     | 1.01              |
| 2:QB:200:ALA:HB1 | 2:QB:232:GLU:CB  | 1.87                     | 1.01              |
| 2:QE:200:ALA:HB1 | 2:QE:232:GLU:CB  | 1.87                     | 1.01              |
| 2:GG:155:HIS:CB  | 2:MG:217:ALA:HB1 | 1.91                     | 1.01              |
| 2:YA:155:HIS:CB  | 2:EB:217:ALA:HB1 | 1.91                     | 1.00              |
| 2:SD:155:HIS:CB  | 2:YD:217:ALA:CB  | 2.39                     | 1.00              |
| 2:CF:155:HIS:CB  | 2:IF:217:ALA:CB  | 2.38                     | 1.00              |
| 2:G:155:HIS:CB   | 2:B:217:ALA:CB   | 2.39                     | 1.00              |
| 2:AA:155:HIS:CB  | 2:GA:217:ALA:CB  | 2.38                     | 1.00              |
| 2:AA:155:HIS:CB  | 2:GA:217:ALA:HB1 | 1.92                     | 1.00              |
| 2:MD:155:HIS:CB  | 2:SD:217:ALA:CB  | 2.39                     | 1.00              |
| 2:KE:200:ALA:HB1 | 2:KE:232:GLU:CB  | 1.87                     | 1.00              |
| 2:UF:155:HIS:CB  | 2:AG:217:ALA:HB1 | 1.92                     | 1.00              |
| 2:CC:155:HIS:CB  | 2:IC:217:ALA:CB  | 2.40                     | 1.00              |
| 2:CF:200:ALA:HB1 | 2:CF:232:GLU:CB  | 1.87                     | 1.00              |
| 2:GA:200:ALA:HB1 | 2:GA:232:GLU:CB  | 1.87                     | 0.99              |
| 2:IC:155:HIS:CB  | 2:OC:217:ALA:HB1 | 1.90                     | 0.99              |
| 2:GD:155:HIS:CB  | 2:MD:217:ALA:HB1 | 1.91                     | 0.99              |
| 2:IF:155:HIS:CB  | 2:OF:217:ALA:HB1 | 1.92                     | 0.99              |
| 2:WE:155:HIS:CB  | 2:CF:217:ALA:CB  | 2.39                     | 0.99              |
| 2:SA:155:HIS:CB  | 2:YA:217:ALA:HB1 | 1.92                     | 0.99              |
| 2:WE:155:HIS:CB  | 2:CF:217:ALA:HB1 | 1.93                     | 0.99              |
| 2:OC:77:LEU:CB   | 2:UC:42:ALA:CA   | 2.41                     | 0.99              |
| 2:EE:200:ALA:HB1 | 2:EE:232:GLU:CB  | 1.87                     | 0.99              |
| 2:MG:200:ALA:HB1 | 2:MG:232:GLU:CB  | 1.87                     | 0.99              |
| 2:EE:155:HIS:CB  | 2:KE:217:ALA:CB  | 2.40                     | 0.98              |
| 2:CF:155:HIS:CB  | 2:IF:217:ALA:HB1 | 1.92                     | 0.98              |
| 2:IF:200:ALA:HB1 | 2:IF:232:GLU:CB  | 1.87                     | 0.98              |
| 2:MG:155:HIS:CB  | 2:SG:217:ALA:CB  | 2.41                     | 0.98              |
| 2:UC:155:HIS:CB  | 2:AD:217:ALA:CB  | 2.41                     | 0.98              |
| 2:G:155:HIS:CB   | 2:B:217:ALA:HB1  | 1.93                     | 0.98              |
| 2:MD:155:HIS:CB  | 2:SD:217:ALA:HB1 | 1.93                     | 0.98              |
| 2:QB:155:HIS:CB  | 2:WB:217:ALA:CB  | 2.42                     | 0.98              |
| 2:MA:155:HIS:CB  | 2:SA:217:ALA:CB  | 2.41                     | 0.97              |
| 2:SD:155:HIS:CB  | 2:YD:217:ALA:HB1 | 1.93                     | 0.97              |
| 2:KE:77:LEU:CB   | 2:QE:42:ALA:CA   | 2.41                     | 0.97              |
| 2:EE:155:HIS:CB  | 2:KE:217:ALA:HB1 | 1.95                     | 0.97              |
| 2:MA:155:HIS:CB  | 2:SA:217:ALA:HB1 | 1.95                     | 0.96              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:MG:155:HIS:CB | 2:SG:217:ALA:HB1 | 1.96                     | 0.95              |
| 2:UC:155:HIS:CB | 2:AD:217:ALA:HB1 | 1.96                     | 0.95              |
| 2:CC:155:HIS:CB | 2:IC:217:ALA:HB1 | 1.94                     | 0.95              |
| 2:AD:77:LEU:CB  | 2:GD:42:ALA:CA   | 2.43                     | 0.95              |
| 2:QB:155:HIS:CB | 2:WB:217:ALA:HB1 | 1.96                     | 0.94              |
| 2:WB:77:LEU:CB  | 2:CC:42:ALA:CA   | 2.45                     | 0.94              |
| 2:IC:77:LEU:CB  | 2:OC:42:ALA:CA   | 2.46                     | 0.94              |
| 2:G:42:ALA:CA   | 2:SG:77:LEU:CB   | 2.45                     | 0.94              |
| 2:GA:77:LEU:CB  | 2:MA:42:ALA:CA   | 2.44                     | 0.94              |
| 2:YA:77:LEU:CB  | 2:EB:42:ALA:CA   | 2.45                     | 0.94              |
| 2:T:77:LEU:CB   | 2:AA:42:ALA:CA   | 2.45                     | 0.93              |
| 2:AG:77:LEU:CB  | 2:GG:42:ALA:CA   | 2.46                     | 0.93              |
| 2:J:77:LEU:CB   | 2:T:42:ALA:CA    | 2.46                     | 0.93              |
| 2:KB:77:LEU:CB  | 2:QB:42:ALA:CA   | 2.46                     | 0.93              |
| 2:OF:77:LEU:CB  | 2:UF:42:ALA:CA   | 2.45                     | 0.93              |
| 2:EB:77:LEU:CB  | 2:KB:42:ALA:CA   | 2.46                     | 0.93              |
| 2:B:77:LEU:CB   | 2:J:42:ALA:CA    | 2.47                     | 0.92              |
| 2:IF:77:LEU:CB  | 2:OF:42:ALA:CA   | 2.47                     | 0.92              |
| 2:YD:77:LEU:CB  | 2:EE:42:ALA:CA   | 2.48                     | 0.91              |
| 2:GD:77:LEU:CB  | 2:MD:42:ALA:CA   | 2.48                     | 0.91              |
| 2:SD:77:LEU:CB  | 2:YD:42:ALA:CA   | 2.50                     | 0.90              |
| 2:GG:77:LEU:CB  | 2:MG:42:ALA:CA   | 2.49                     | 0.90              |
| 2:QE:77:LEU:CB  | 2:WE:42:ALA:CA   | 2.48                     | 0.90              |
| 2:UF:77:LEU:CB  | 2:AG:42:ALA:CA   | 2.49                     | 0.90              |
| 2:AA:77:LEU:CB  | 2:GA:42:ALA:CA   | 2.48                     | 0.90              |
| 2:SA:77:LEU:CB  | 2:YA:42:ALA:CA   | 2.48                     | 0.89              |
| 2:CC:77:LEU:CB  | 2:IC:42:ALA:CA   | 2.51                     | 0.89              |
| 2:MD:77:LEU:CB  | 2:SD:42:ALA:CA   | 2.51                     | 0.88              |
| 2:G:77:LEU:CB   | 2:B:42:ALA:CA    | 2.51                     | 0.88              |
| 2:CF:77:LEU:CB  | 2:IF:42:ALA:CA   | 2.49                     | 0.88              |
| 2:EE:77:LEU:CB  | 2:KE:42:ALA:CA   | 2.51                     | 0.88              |
| 2:AA:218:VAL:C  | 2:AA:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:OC:218:VAL:C  | 2:OC:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:G:218:VAL:C   | 2:G:226:ALA:HB2  | 2.00                     | 0.87              |
| 2:SA:218:VAL:C  | 2:SA:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:WB:218:VAL:C  | 2:WB:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:SD:218:VAL:C  | 2:SD:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:IF:218:VAL:C  | 2:IF:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:B:218:VAL:C   | 2:B:226:ALA:HB2  | 2.00                     | 0.87              |
| 2:AD:218:VAL:C  | 2:AD:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:GD:218:VAL:C  | 2:GD:226:ALA:HB2 | 2.00                     | 0.87              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:YD:218:VAL:C  | 2:YD:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:OF:218:VAL:C  | 2:OF:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:EB:218:VAL:C  | 2:EB:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:KB:218:VAL:C  | 2:KB:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:SG:218:VAL:C  | 2:SG:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:KE:218:VAL:C  | 2:KE:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:CF:218:VAL:C  | 2:CF:226:ALA:HB2 | 2.00                     | 0.87              |
| 2:MG:218:VAL:C  | 2:MG:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:J:218:VAL:C   | 2:J:226:ALA:HB2  | 2.00                     | 0.86              |
| 2:MA:218:VAL:C  | 2:MA:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:IC:218:VAL:C  | 2:IC:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:UC:77:LEU:CB  | 2:AD:42:ALA:CA   | 2.53                     | 0.86              |
| 2:WE:77:LEU:CB  | 2:CF:42:ALA:CA   | 2.51                     | 0.86              |
| 2:UF:218:VAL:C  | 2:UF:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:EE:218:VAL:C  | 2:EE:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:GA:218:VAL:C  | 2:GA:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:CC:218:VAL:C  | 2:CC:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:QE:218:VAL:C  | 2:QE:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:AG:218:VAL:C  | 2:AG:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:T:218:VAL:C   | 2:T:226:ALA:HB2  | 2.00                     | 0.86              |
| 2:WE:218:VAL:C  | 2:WE:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:QB:218:VAL:C  | 2:QB:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:MG:77:LEU:CB  | 2:SG:42:ALA:CA   | 2.52                     | 0.86              |
| 2:MD:218:VAL:C  | 2:MD:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:UC:218:VAL:C  | 2:UC:226:ALA:HB2 | 2.00                     | 0.86              |
| 2:YA:218:VAL:C  | 2:YA:226:ALA:HB2 | 2.00                     | 0.85              |
| 2:QB:77:LEU:CB  | 2:WB:42:ALA:CA   | 2.52                     | 0.85              |
| 2:GG:218:VAL:C  | 2:GG:226:ALA:HB2 | 2.00                     | 0.85              |
| 2:MA:77:LEU:CB  | 2:SA:42:ALA:CA   | 2.54                     | 0.83              |
| 3:LE:258:GLU:CB | 4:UE:102:ASN:CB  | 2.65                     | 0.75              |
| 2:MA:143:ALA:CB | 2:SA:205:LEU:O   | 2.32                     | 0.75              |
| 2:GA:143:ALA:CB | 2:MA:205:LEU:O   | 2.32                     | 0.75              |
| 2:YA:143:ALA:CB | 2:EB:205:LEU:O   | 2.34                     | 0.75              |
| 2:EB:143:ALA:CB | 2:KB:205:LEU:O   | 2.33                     | 0.75              |
| 2:QB:143:ALA:CB | 2:WB:205:LEU:O   | 2.34                     | 0.75              |
| 2:WB:143:ALA:CB | 2:CC:205:LEU:O   | 2.33                     | 0.75              |
| 2:AA:143:ALA:CB | 2:GA:205:LEU:O   | 2.33                     | 0.74              |
| 3:ZA:258:GLU:CB | 4:IB:102:ASN:CB  | 2.65                     | 0.74              |
| 3:JC:258:GLU:CB | 4:SC:102:ASN:CB  | 2.66                     | 0.74              |
| 2:J:143:ALA:CB  | 2:T:205:LEU:O    | 2.33                     | 0.74              |
| 2:KB:143:ALA:CB | 2:QB:205:LEU:O   | 2.31                     | 0.74              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:IC:143:ALA:CB  | 2:OC:205:LEU:O  | 2.34                     | 0.74              |
| 2:B:143:ALA:CB   | 2:J:205:LEU:O   | 2.33                     | 0.74              |
| 2:CC:143:ALA:CB  | 2:IC:205:LEU:O  | 2.33                     | 0.74              |
| 2:UC:143:ALA:CB  | 2:AD:205:LEU:O  | 2.33                     | 0.74              |
| 2:T:143:ALA:CB   | 2:AA:205:LEU:O  | 2.32                     | 0.74              |
| 2:OC:143:ALA:CB  | 2:UC:205:LEU:O  | 2.31                     | 0.74              |
| 2:G:205:LEU:O    | 2:SG:143:ALA:CB | 2.33                     | 0.73              |
| 2:SA:143:ALA:CB  | 2:YA:205:LEU:O  | 2.33                     | 0.73              |
| 2:AD:143:ALA:CB  | 2:GD:205:LEU:O  | 2.32                     | 0.73              |
| 2:OC:143:ALA:HB3 | 2:UC:205:LEU:O  | 1.88                     | 0.73              |
| 2:G:143:ALA:CB   | 2:B:205:LEU:O   | 2.33                     | 0.73              |
| 3:K:258:GLU:CB   | 4:Y:102:ASN:CB  | 2.66                     | 0.73              |
| 2:GD:143:ALA:CB  | 2:MD:205:LEU:O  | 2.33                     | 0.73              |
| 3:JF:258:GLU:CB  | 4:SF:102:ASN:CB | 2.66                     | 0.73              |
| 3:XB:258:GLU:CB  | 4:GC:102:ASN:CB | 2.67                     | 0.72              |
| 3:BD:258:GLU:CB  | 4:KD:102:ASN:CB | 2.67                     | 0.72              |
| 2:MD:143:ALA:CB  | 2:SD:205:LEU:O  | 2.32                     | 0.72              |
| 3:FB:258:GLU:CB  | 4:OB:102:ASN:CB | 2.68                     | 0.72              |
| 4:Q:102:ASN:CB   | 3:TG:258:GLU:CB | 2.67                     | 0.72              |
| 2:KB:143:ALA:HB3 | 2:QB:205:LEU:O  | 1.90                     | 0.72              |
| 2:MG:143:ALA:CB  | 2:SG:205:LEU:O  | 2.34                     | 0.72              |
| 2:SD:143:ALA:CB  | 2:YD:205:LEU:O  | 2.33                     | 0.72              |
| 2:AG:143:ALA:CB  | 2:GG:205:LEU:O  | 2.32                     | 0.72              |
| 2:GG:143:ALA:CB  | 2:MG:205:LEU:O  | 2.32                     | 0.72              |
| 3:HA:258:GLU:CB  | 4:QA:102:ASN:CB | 2.67                     | 0.72              |
| 3:PC:258:GLU:CB  | 4:YC:102:ASN:CB | 2.67                     | 0.72              |
| 3:BG:258:GLU:CB  | 4:KG:102:ASN:CB | 2.68                     | 0.72              |
| 3:V:258:GLU:CB   | 4:EA:102:ASN:CB | 2.68                     | 0.72              |
| 2:YD:143:ALA:CB  | 2:EE:205:LEU:O  | 2.32                     | 0.72              |
| 2:KE:143:ALA:HB3 | 2:QE:205:LEU:O  | 1.90                     | 0.72              |
| 3:PF:258:GLU:CB  | 4:YF:102:ASN:CB | 2.68                     | 0.72              |
| 3:BA:258:GLU:CB  | 4:KA:102:ASN:CB | 2.68                     | 0.71              |
| 2:AD:143:ALA:HB3 | 2:GD:205:LEU:O  | 1.90                     | 0.71              |
| 3:C:258:GLU:CB   | 4:R:102:ASN:CB  | 2.68                     | 0.71              |
| 2:IF:143:ALA:CB  | 2:OF:205:LEU:O  | 2.34                     | 0.71              |
| 2:UF:143:ALA:CB  | 2:AG:205:LEU:O  | 2.33                     | 0.71              |
| 2:GA:143:ALA:HB3 | 2:MA:205:LEU:O  | 1.91                     | 0.71              |
| 2:EE:143:ALA:CB  | 2:KE:205:LEU:O  | 2.34                     | 0.71              |
| 2:B:242:VAL:HA   | 2:B:324:GLY:HA2 | 1.73                     | 0.71              |
| 3:TA:258:GLU:CB  | 4:CB:102:ASN:CB | 2.68                     | 0.71              |
| 2:OF:143:ALA:CB  | 2:UF:205:LEU:O  | 2.32                     | 0.71              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:UF:242:VAL:HA | 2:UF:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:AG:242:VAL:HA | 2:AG:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:GG:242:VAL:HA | 2:GG:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:SG:242:VAL:HA | 2:SG:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:G:242:VAL:HA  | 2:G:324:GLY:HA2  | 1.73                     | 0.71              |
| 2:J:242:VAL:HA  | 2:J:324:GLY:HA2  | 1.73                     | 0.71              |
| 2:T:242:VAL:HA  | 2:T:324:GLY:HA2  | 1.73                     | 0.71              |
| 2:AA:242:VAL:HA | 2:AA:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:YA:242:VAL:HA | 2:YA:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:KB:242:VAL:HA | 2:KB:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:WB:242:VAL:HA | 2:WB:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:IF:242:VAL:HA | 2:IF:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:OF:242:VAL:HA | 2:OF:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:MG:242:VAL:HA | 2:MG:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:GA:242:VAL:HA | 2:GA:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:MA:242:VAL:HA | 2:MA:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:QB:242:VAL:HA | 2:QB:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:IC:242:VAL:HA | 2:IC:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:UC:242:VAL:HA | 2:UC:324:GLY:HA2 | 1.73                     | 0.71              |
| 3:TD:258:GLU:CB | 4:CE:102:ASN:CB  | 2.69                     | 0.71              |
| 2:QE:242:VAL:HA | 2:QE:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:WE:242:VAL:HA | 2:WE:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:CF:242:VAL:HA | 2:CF:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:SA:242:VAL:HA | 2:SA:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:EB:242:VAL:HA | 2:EB:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:CC:242:VAL:HA | 2:CC:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:GD:242:VAL:HA | 2:GD:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:YD:242:VAL:HA | 2:YD:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:KE:242:VAL:HA | 2:KE:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:WE:143:ALA:CB | 2:CF:205:LEU:O   | 2.32                     | 0.71              |
| 2:CF:143:ALA:CB | 2:IF:205:LEU:O   | 2.33                     | 0.71              |
| 2:OC:242:VAL:HA | 2:OC:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:AD:242:VAL:HA | 2:AD:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:MD:242:VAL:HA | 2:MD:324:GLY:HA2 | 1.73                     | 0.71              |
| 2:SD:242:VAL:HA | 2:SD:324:GLY:HA2 | 1.73                     | 0.71              |
| 3:RE:258:GLU:CB | 4:AF:102:ASN:CB  | 2.69                     | 0.71              |
| 2:EE:242:VAL:HA | 2:EE:324:GLY:HA2 | 1.73                     | 0.70              |
| 2:KE:143:ALA:CB | 2:QE:205:LEU:O   | 2.33                     | 0.70              |
| 2:QE:143:ALA:CB | 2:WE:205:LEU:O   | 2.33                     | 0.70              |
| 3:VF:258:GLU:CB | 4:EG:102:ASN:CB  | 2.70                     | 0.70              |
| 3:HD:258:GLU:CB | 4:QD:102:ASN:CB  | 2.69                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:143:ALA:HB3  | 2:AA:205:LEU:O   | 1.91                     | 0.70              |
| 3:DF:258:GLU:CB  | 4:MF:102:ASN:CB  | 2.69                     | 0.70              |
| 3:RB:258:GLU:CB  | 4:AC:102:ASN:CB  | 2.70                     | 0.69              |
| 3:DC:258:GLU:CB  | 4:MC:102:ASN:CB  | 2.70                     | 0.69              |
| 3:FE:258:GLU:CB  | 4:OE:102:ASN:CB  | 2.69                     | 0.69              |
| 3:NG:258:GLU:CB  | 4:WG:102:ASN:CB  | 2.70                     | 0.69              |
| 2:EB:143:ALA:HB3 | 2:KB:205:LEU:O   | 1.92                     | 0.69              |
| 2:OC:155:HIS:CB  | 2:UC:217:ALA:HB2 | 2.22                     | 0.69              |
| 2:AG:143:ALA:HB3 | 2:GG:205:LEU:O   | 1.92                     | 0.69              |
| 2:YD:143:ALA:HB3 | 2:EE:205:LEU:O   | 1.92                     | 0.69              |
| 3:HG:258:GLU:CB  | 4:QG:102:ASN:CB  | 2.70                     | 0.69              |
| 3:M:258:GLU:CB   | 4:H:102:ASN:CB   | 2.70                     | 0.69              |
| 2:OF:143:ALA:HB3 | 2:UF:205:LEU:O   | 1.91                     | 0.69              |
| 2:WB:143:ALA:HB3 | 2:CC:205:LEU:O   | 1.92                     | 0.69              |
| 2:J:143:ALA:HB3  | 2:T:205:LEU:O    | 1.93                     | 0.68              |
| 2:GD:143:ALA:HB3 | 2:MD:205:LEU:O   | 1.93                     | 0.68              |
| 2:G:205:LEU:O    | 2:SG:143:ALA:HB3 | 1.92                     | 0.68              |
| 3:ZD:258:GLU:CB  | 4:IE:102:ASN:CB  | 2.70                     | 0.68              |
| 2:WE:143:ALA:HB3 | 2:CF:205:LEU:O   | 1.94                     | 0.68              |
| 2:GG:143:ALA:HB3 | 2:MG:205:LEU:O   | 1.93                     | 0.68              |
| 2:B:143:ALA:HB3  | 2:J:205:LEU:O    | 1.93                     | 0.68              |
| 2:QE:143:ALA:HB3 | 2:WE:205:LEU:O   | 1.92                     | 0.68              |
| 2:SA:143:ALA:HB3 | 2:YA:205:LEU:O   | 1.94                     | 0.68              |
| 3:LB:258:GLU:CB  | 4:UB:102:ASN:CB  | 2.71                     | 0.68              |
| 2:UF:143:ALA:HB3 | 2:AG:205:LEU:O   | 1.93                     | 0.68              |
| 2:G:143:ALA:HB3  | 2:B:205:LEU:O    | 1.94                     | 0.68              |
| 2:AA:143:ALA:HB3 | 2:GA:205:LEU:O   | 1.94                     | 0.68              |
| 3:VC:258:GLU:CB  | 4:ED:102:ASN:CB  | 2.71                     | 0.68              |
| 3:XE:258:GLU:CB  | 4:GF:102:ASN:CB  | 2.72                     | 0.68              |
| 2:AD:155:HIS:CB  | 2:GD:217:ALA:HB2 | 2.24                     | 0.68              |
| 3:ND:258:GLU:CB  | 4:WD:102:ASN:CB  | 2.72                     | 0.67              |
| 2:MA:143:ALA:HB3 | 2:SA:205:LEU:O   | 1.95                     | 0.67              |
| 2:MD:143:ALA:HB3 | 2:SD:205:LEU:O   | 1.94                     | 0.67              |
| 2:KE:155:HIS:CB  | 2:QE:217:ALA:HB2 | 2.22                     | 0.67              |
| 2:KB:68:ALA:HB1  | 2:QB:47:ILE:O    | 1.95                     | 0.67              |
| 2:IC:143:ALA:HB3 | 2:OC:205:LEU:O   | 1.93                     | 0.67              |
| 2:IF:143:ALA:HB3 | 2:OF:205:LEU:O   | 1.94                     | 0.67              |
| 2:CF:143:ALA:HB3 | 2:IF:205:LEU:O   | 1.93                     | 0.67              |
| 2:YA:143:ALA:HB3 | 2:EB:205:LEU:O   | 1.94                     | 0.66              |
| 2:SD:143:ALA:HB3 | 2:YD:205:LEU:O   | 1.94                     | 0.66              |
| 2:WB:155:HIS:CB  | 2:CC:217:ALA:HB2 | 2.25                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:MG:143:ALA:HB3 | 2:SG:205:LEU:O   | 1.96                     | 0.66              |
| 2:GA:155:HIS:CB  | 2:MA:217:ALA:HB2 | 2.24                     | 0.66              |
| 2:CC:143:ALA:HB3 | 2:IC:205:LEU:O   | 1.95                     | 0.66              |
| 2:YA:155:HIS:CB  | 2:EB:217:ALA:HB2 | 2.25                     | 0.66              |
| 4:BB:64:LEU:HA   | 4:BB:101:ILE:HA  | 1.78                     | 0.66              |
| 2:KB:74:ASN:CA   | 2:QB:42:ALA:O    | 2.44                     | 0.66              |
| 2:UC:143:ALA:HB3 | 2:AD:205:LEU:O   | 1.95                     | 0.66              |
| 2:MD:219:ARG:N   | 2:MD:226:ALA:HB2 | 2.11                     | 0.66              |
| 4:TB:64:LEU:HA   | 4:TB:101:ILE:HA  | 1.78                     | 0.66              |
| 4:ZB:64:LEU:HA   | 4:ZB:101:ILE:HA  | 1.78                     | 0.66              |
| 2:GD:219:ARG:N   | 2:GD:226:ALA:HB2 | 2.11                     | 0.66              |
| 2:AG:219:ARG:N   | 2:AG:226:ALA:HB2 | 2.11                     | 0.66              |
| 2:GG:219:ARG:N   | 2:GG:226:ALA:HB2 | 2.11                     | 0.66              |
| 4:NB:64:LEU:HA   | 4:NB:101:ILE:HA  | 1.78                     | 0.66              |
| 4:FC:64:LEU:HA   | 4:FC:101:ILE:HA  | 1.78                     | 0.66              |
| 2:IC:155:HIS:CB  | 2:OC:217:ALA:HB2 | 2.25                     | 0.66              |
| 4:RC:64:LEU:HA   | 4:RC:101:ILE:HA  | 1.78                     | 0.66              |
| 2:QE:219:ARG:N   | 2:QE:226:ALA:HB2 | 2.11                     | 0.66              |
| 2:WE:219:ARG:N   | 2:WE:226:ALA:HB2 | 2.11                     | 0.66              |
| 2:J:219:ARG:N    | 2:J:226:ALA:HB2  | 2.11                     | 0.65              |
| 2:CC:219:ARG:N   | 2:CC:226:ALA:HB2 | 2.11                     | 0.65              |
| 2:EE:143:ALA:HB3 | 2:KE:205:LEU:O   | 1.95                     | 0.65              |
| 2:T:219:ARG:N    | 2:T:226:ALA:HB2  | 2.11                     | 0.65              |
| 4:PA:64:LEU:HA   | 4:PA:101:ILE:HA  | 1.78                     | 0.65              |
| 4:VA:64:LEU:HA   | 4:VA:101:ILE:HA  | 1.78                     | 0.65              |
| 4:LC:64:LEU:HA   | 4:LC:101:ILE:HA  | 1.78                     | 0.65              |
| 2:SD:219:ARG:N   | 2:SD:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:RF:64:LEU:HA   | 4:RF:101:ILE:HA  | 1.78                     | 0.65              |
| 2:MG:219:ARG:N   | 2:MG:226:ALA:HB2 | 2.11                     | 0.65              |
| 2:B:219:ARG:N    | 2:B:226:ALA:HB2  | 2.11                     | 0.65              |
| 2:SA:219:ARG:N   | 2:SA:226:ALA:HB2 | 2.11                     | 0.65              |
| 2:EB:155:HIS:CB  | 2:KB:217:ALA:HB2 | 2.26                     | 0.65              |
| 2:IC:219:ARG:N   | 2:IC:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:ZE:64:LEU:HA   | 4:ZE:101:ILE:HA  | 1.78                     | 0.65              |
| 2:UF:219:ARG:N   | 2:UF:226:ALA:HB2 | 2.11                     | 0.65              |
| 3:NA:258:GLU:CB  | 4:WA:102:ASN:CB  | 2.74                     | 0.65              |
| 2:YA:219:ARG:N   | 2:YA:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:HB:64:LEU:HA   | 4:HB:101:ILE:HA  | 1.78                     | 0.65              |
| 2:AD:219:ARG:N   | 2:AD:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:DD:64:LEU:HA   | 4:DD:101:ILE:HA  | 1.78                     | 0.65              |
| 2:KE:219:ARG:N   | 2:KE:226:ALA:HB2 | 2.11                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:CF:219:ARG:N   | 2:CF:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:DA:64:LEU:HA   | 4:DA:101:ILE:HA  | 1.78                     | 0.65              |
| 2:WB:219:ARG:N   | 2:WB:226:ALA:HB2 | 2.11                     | 0.65              |
| 2:G:217:ALA:HB2  | 2:SG:155:HIS:CB  | 2.25                     | 0.65              |
| 4:LF:64:LEU:HA   | 4:LF:101:ILE:HA  | 1.78                     | 0.65              |
| 2:T:155:HIS:CB   | 2:AA:217:ALA:HB2 | 2.26                     | 0.65              |
| 4:X:64:LEU:HA    | 4:X:101:ILE:HA   | 1.78                     | 0.65              |
| 4:JA:64:LEU:HA   | 4:JA:101:ILE:HA  | 1.78                     | 0.65              |
| 2:QB:143:ALA:HB3 | 2:WB:205:LEU:O   | 1.96                     | 0.65              |
| 4:JG:64:LEU:HA   | 4:JG:101:ILE:HA  | 1.78                     | 0.65              |
| 2:G:25:VAL:O     | 2:G:29:LEU:CB    | 2.45                     | 0.65              |
| 2:GA:25:VAL:O    | 2:GA:29:LEU:CB   | 2.45                     | 0.65              |
| 2:OC:219:ARG:N   | 2:OC:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:XC:64:LEU:HA   | 4:XC:101:ILE:HA  | 1.78                     | 0.65              |
| 2:IF:155:HIS:CB  | 2:OF:217:ALA:HB2 | 2.26                     | 0.65              |
| 4:DG:64:LEU:HA   | 4:DG:101:ILE:HA  | 1.78                     | 0.65              |
| 2:AA:219:ARG:N   | 2:AA:226:ALA:HB2 | 2.11                     | 0.65              |
| 2:EB:219:ARG:N   | 2:EB:226:ALA:HB2 | 2.11                     | 0.65              |
| 2:YD:219:ARG:N   | 2:YD:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:TE:64:LEU:HA   | 4:TE:101:ILE:HA  | 1.78                     | 0.65              |
| 2:IF:219:ARG:N   | 2:IF:226:ALA:HB2 | 2.11                     | 0.65              |
| 2:G:219:ARG:N    | 2:G:226:ALA:HB2  | 2.11                     | 0.65              |
| 2:MA:219:ARG:N   | 2:MA:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:JD:64:LEU:HA   | 4:JD:101:ILE:HA  | 1.78                     | 0.65              |
| 4:PD:64:LEU:HA   | 4:PD:101:ILE:HA  | 1.78                     | 0.65              |
| 2:EE:219:ARG:N   | 2:EE:226:ALA:HB2 | 2.11                     | 0.65              |
| 4:HE:64:LEU:HA   | 4:HE:101:ILE:HA  | 1.78                     | 0.65              |
| 2:SG:25:VAL:O    | 2:SG:29:LEU:CB   | 2.45                     | 0.65              |
| 4:VG:64:LEU:HA   | 4:VG:101:ILE:HA  | 1.78                     | 0.65              |
| 2:AA:25:VAL:O    | 2:AA:29:LEU:CB   | 2.45                     | 0.64              |
| 2:MA:25:VAL:O    | 2:MA:29:LEU:CB   | 2.45                     | 0.64              |
| 2:QB:219:ARG:N   | 2:QB:226:ALA:HB2 | 2.11                     | 0.64              |
| 2:SG:219:ARG:N   | 2:SG:226:ALA:HB2 | 2.11                     | 0.64              |
| 2:B:25:VAL:O     | 2:B:29:LEU:CB    | 2.45                     | 0.64              |
| 2:KB:25:VAL:O    | 2:KB:29:LEU:CB   | 2.45                     | 0.64              |
| 2:QB:25:VAL:O    | 2:QB:29:LEU:CB   | 2.45                     | 0.64              |
| 2:UC:219:ARG:N   | 2:UC:226:ALA:HB2 | 2.11                     | 0.64              |
| 2:OF:219:ARG:N   | 2:OF:226:ALA:HB2 | 2.11                     | 0.64              |
| 4:P:64:LEU:HA    | 4:P:101:ILE:HA   | 1.78                     | 0.64              |
| 4:E:64:LEU:HA    | 4:E:101:ILE:HA   | 1.78                     | 0.64              |
| 2:J:155:HIS:CB   | 2:T:217:ALA:HB2  | 2.26                     | 0.64              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:O:64:LEU:HA   | 4:O:101:ILE:HA   | 1.78                     | 0.64              |
| 2:MD:25:VAL:O   | 2:MD:29:LEU:CB   | 2.45                     | 0.64              |
| 2:SD:25:VAL:O   | 2:SD:29:LEU:CB   | 2.45                     | 0.64              |
| 2:EE:25:VAL:O   | 2:EE:29:LEU:CB   | 2.45                     | 0.64              |
| 2:UF:25:VAL:O   | 2:UF:29:LEU:CB   | 2.45                     | 0.64              |
| 2:EB:25:VAL:O   | 2:EB:29:LEU:CB   | 2.45                     | 0.64              |
| 2:OC:68:ALA:HB1 | 2:UC:47:ILE:O    | 1.98                     | 0.64              |
| 2:GD:25:VAL:O   | 2:GD:29:LEU:CB   | 2.45                     | 0.64              |
| 2:YD:25:VAL:O   | 2:YD:29:LEU:CB   | 2.45                     | 0.64              |
| 4:BE:64:LEU:HA  | 4:BE:101:ILE:HA  | 1.78                     | 0.64              |
| 2:KE:25:VAL:O   | 2:KE:29:LEU:CB   | 2.45                     | 0.64              |
| 2:QE:25:VAL:O   | 2:QE:29:LEU:CB   | 2.45                     | 0.64              |
| 2:KB:219:ARG:N  | 2:KB:226:ALA:HB2 | 2.11                     | 0.64              |
| 2:UC:25:VAL:O   | 2:UC:29:LEU:CB   | 2.45                     | 0.64              |
| 2:AD:25:VAL:O   | 2:AD:29:LEU:CB   | 2.45                     | 0.64              |
| 2:OF:25:VAL:O   | 2:OF:29:LEU:CB   | 2.45                     | 0.64              |
| 2:SA:25:VAL:O   | 2:SA:29:LEU:CB   | 2.45                     | 0.64              |
| 2:WB:25:VAL:O   | 2:WB:29:LEU:CB   | 2.45                     | 0.64              |
| 2:WE:25:VAL:O   | 2:WE:29:LEU:CB   | 2.45                     | 0.64              |
| 2:OC:25:VAL:O   | 2:OC:29:LEU:CB   | 2.45                     | 0.64              |
| 4:VD:64:LEU:HA  | 4:VD:101:ILE:HA  | 1.78                     | 0.64              |
| 2:CF:25:VAL:O   | 2:CF:29:LEU:CB   | 2.45                     | 0.64              |
| 2:MG:25:VAL:O   | 2:MG:29:LEU:CB   | 2.45                     | 0.64              |
| 2:GA:219:ARG:N  | 2:GA:226:ALA:HB2 | 2.11                     | 0.64              |
| 3:NA:105:ILE:HA | 3:NA:179:TYR:HA  | 1.80                     | 0.64              |
| 2:IF:25:VAL:O   | 2:IF:29:LEU:CB   | 2.45                     | 0.64              |
| 2:AG:25:VAL:O   | 2:AG:29:LEU:CB   | 2.45                     | 0.64              |
| 2:T:25:VAL:O    | 2:T:29:LEU:CB    | 2.45                     | 0.64              |
| 3:TA:105:ILE:HA | 3:TA:179:TYR:HA  | 1.80                     | 0.64              |
| 2:IC:25:VAL:O   | 2:IC:29:LEU:CB   | 2.45                     | 0.64              |
| 4:FF:64:LEU:HA  | 4:FF:101:ILE:HA  | 1.78                     | 0.64              |
| 3:HG:105:ILE:HA | 3:HG:179:TYR:HA  | 1.80                     | 0.64              |
| 3:TG:105:ILE:HA | 3:TG:179:TYR:HA  | 1.80                     | 0.64              |
| 3:C:105:ILE:HA  | 3:C:179:TYR:HA   | 1.80                     | 0.64              |
| 2:J:25:VAL:O    | 2:J:29:LEU:CB    | 2.45                     | 0.64              |
| 3:V:105:ILE:HA  | 3:V:179:TYR:HA   | 1.80                     | 0.64              |
| 3:BA:105:ILE:HA | 3:BA:179:TYR:HA  | 1.80                     | 0.64              |
| 3:HA:105:ILE:HA | 3:HA:179:TYR:HA  | 1.80                     | 0.64              |
| 4:XF:64:LEU:HA  | 4:XF:101:ILE:HA  | 1.78                     | 0.64              |
| 3:NG:105:ILE:HA | 3:NG:179:TYR:HA  | 1.80                     | 0.64              |
| 3:M:105:ILE:HA  | 3:M:179:TYR:HA   | 1.80                     | 0.63              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:ZA:105:ILE:HA | 3:ZA:179:TYR:HA  | 1.80                     | 0.63              |
| 2:CC:25:VAL:O   | 2:CC:29:LEU:CB   | 2.45                     | 0.63              |
| 3:BG:105:ILE:HA | 3:BG:179:TYR:HA  | 1.80                     | 0.63              |
| 3:K:105:ILE:HA  | 3:K:179:TYR:HA   | 1.80                     | 0.63              |
| 2:YA:77:LEU:CB  | 2:EB:42:ALA:O    | 2.46                     | 0.63              |
| 3:FB:105:ILE:HA | 3:FB:179:TYR:HA  | 1.80                     | 0.63              |
| 2:B:155:HIS:CB  | 2:J:217:ALA:HB2  | 2.27                     | 0.63              |
| 2:YA:25:VAL:O   | 2:YA:29:LEU:CB   | 2.45                     | 0.63              |
| 3:JF:90:HIS:N   | 3:JF:195:PRO:O   | 2.31                     | 0.63              |
| 3:VF:105:ILE:HA | 3:VF:179:TYR:HA  | 1.80                     | 0.63              |
| 3:NG:90:HIS:N   | 3:NG:195:PRO:O   | 2.31                     | 0.63              |
| 3:LB:105:ILE:HA | 3:LB:179:TYR:HA  | 1.80                     | 0.63              |
| 4:NE:64:LEU:HA  | 4:NE:101:ILE:HA  | 1.78                     | 0.63              |
| 3:PF:105:ILE:HA | 3:PF:179:TYR:HA  | 1.80                     | 0.63              |
| 3:M:90:HIS:N    | 3:M:195:PRO:O    | 2.31                     | 0.63              |
| 3:RB:105:ILE:HA | 3:RB:179:TYR:HA  | 1.80                     | 0.63              |
| 3:XE:90:HIS:N   | 3:XE:195:PRO:O   | 2.31                     | 0.63              |
| 2:GG:25:VAL:O   | 2:GG:29:LEU:CB   | 2.45                     | 0.63              |
| 4:PG:64:LEU:HA  | 4:PG:101:ILE:HA  | 1.78                     | 0.63              |
| 2:CF:219:ARG:HA | 2:CF:226:ALA:CB  | 2.29                     | 0.63              |
| 3:JF:105:ILE:HA | 3:JF:179:TYR:HA  | 1.80                     | 0.63              |
| 2:AG:155:HIS:CB | 2:GG:217:ALA:HB2 | 2.26                     | 0.63              |
| 3:BG:90:HIS:N   | 3:BG:195:PRO:O   | 2.31                     | 0.63              |
| 3:K:90:HIS:N    | 3:K:195:PRO:O    | 2.31                     | 0.63              |
| 3:XB:105:ILE:HA | 3:XB:179:TYR:HA  | 1.80                     | 0.63              |
| 2:OC:74:ASN:CA  | 2:UC:42:ALA:O    | 2.47                     | 0.63              |
| 2:QE:219:ARG:HA | 2:QE:226:ALA:CB  | 2.29                     | 0.63              |
| 2:WE:219:ARG:HA | 2:WE:226:ALA:CB  | 2.29                     | 0.63              |
| 2:IF:219:ARG:HA | 2:IF:226:ALA:CB  | 2.29                     | 0.63              |
| 2:GD:155:HIS:CB | 2:MD:217:ALA:HB2 | 2.28                     | 0.63              |
| 3:ND:105:ILE:HA | 3:ND:179:TYR:HA  | 1.80                     | 0.63              |
| 2:KE:219:ARG:HA | 2:KE:226:ALA:CB  | 2.29                     | 0.63              |
| 3:DF:105:ILE:HA | 3:DF:179:TYR:HA  | 1.80                     | 0.63              |
| 2:OF:219:ARG:HA | 2:OF:226:ALA:CB  | 2.29                     | 0.63              |
| 2:EE:219:ARG:HA | 2:EE:226:ALA:CB  | 2.29                     | 0.62              |
| 3:XE:105:ILE:HA | 3:XE:179:TYR:HA  | 1.80                     | 0.62              |
| 2:MD:219:ARG:HA | 2:MD:226:ALA:CB  | 2.29                     | 0.62              |
| 2:SD:219:ARG:HA | 2:SD:226:ALA:CB  | 2.29                     | 0.62              |
| 3:TD:106:HIS:N  | 3:TD:178:GLU:O   | 2.32                     | 0.62              |
| 3:LE:90:HIS:N   | 3:LE:195:PRO:O   | 2.31                     | 0.62              |
| 2:MA:68:ALA:HB1 | 2:SA:47:ILE:O    | 1.99                     | 0.62              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:DC:105:ILE:HA | 3:DC:179:TYR:HA  | 1.80                     | 0.62              |
| 2:UC:219:ARG:HA | 2:UC:226:ALA:CB  | 2.29                     | 0.62              |
| 2:AD:219:ARG:HA | 2:AD:226:ALA:CB  | 2.29                     | 0.62              |
| 2:GD:219:ARG:HA | 2:GD:226:ALA:CB  | 2.29                     | 0.62              |
| 2:YD:219:ARG:HA | 2:YD:226:ALA:CB  | 2.29                     | 0.62              |
| 3:LE:106:HIS:N  | 3:LE:178:GLU:O   | 2.32                     | 0.62              |
| 2:IF:77:LEU:CB  | 2:OF:42:ALA:O    | 2.47                     | 0.62              |
| 2:OF:155:HIS:CB | 2:UF:217:ALA:HB2 | 2.26                     | 0.62              |
| 3:PF:90:HIS:N   | 3:PF:195:PRO:O   | 2.31                     | 0.62              |
| 2:UF:219:ARG:HA | 2:UF:226:ALA:CB  | 2.29                     | 0.62              |
| 2:AA:155:HIS:CB | 2:GA:217:ALA:HB2 | 2.28                     | 0.62              |
| 3:VC:106:HIS:N  | 3:VC:178:GLU:O   | 2.32                     | 0.62              |
| 3:ND:106:HIS:N  | 3:ND:178:GLU:O   | 2.32                     | 0.62              |
| 3:FE:105:ILE:HA | 3:FE:179:TYR:HA  | 1.80                     | 0.62              |
| 3:DC:106:HIS:N  | 3:DC:178:GLU:O   | 2.32                     | 0.62              |
| 2:OC:219:ARG:HA | 2:OC:226:ALA:CB  | 2.29                     | 0.62              |
| 3:VC:105:ILE:HA | 3:VC:179:TYR:HA  | 1.80                     | 0.62              |
| 3:BD:106:HIS:N  | 3:BD:178:GLU:O   | 2.32                     | 0.62              |
| 3:BA:90:HIS:N   | 3:BA:195:PRO:O   | 2.31                     | 0.62              |
| 2:IC:219:ARG:HA | 2:IC:226:ALA:CB  | 2.29                     | 0.62              |
| 3:JC:105:ILE:HA | 3:JC:179:TYR:HA  | 1.80                     | 0.62              |
| 3:BD:105:ILE:HA | 3:BD:179:TYR:HA  | 1.80                     | 0.62              |
| 3:RE:105:ILE:HA | 3:RE:179:TYR:HA  | 1.80                     | 0.62              |
| 2:WE:19:GLU:HA  | 2:WE:22:ALA:HB3  | 1.82                     | 0.62              |
| 3:DF:106:HIS:N  | 3:DF:178:GLU:O   | 2.32                     | 0.62              |
| 2:T:19:GLU:HA   | 2:T:22:ALA:HB3   | 1.82                     | 0.62              |
| 2:AA:19:GLU:HA  | 2:AA:22:ALA:HB3  | 1.82                     | 0.62              |
| 2:GA:219:ARG:HA | 2:GA:226:ALA:CB  | 2.29                     | 0.62              |
| 2:YA:19:GLU:HA  | 2:YA:22:ALA:HB3  | 1.82                     | 0.62              |
| 3:ZD:105:ILE:HA | 3:ZD:179:TYR:HA  | 1.80                     | 0.62              |
| 3:FE:106:HIS:N  | 3:FE:178:GLU:O   | 2.32                     | 0.62              |
| 3:LE:105:ILE:HA | 3:LE:179:TYR:HA  | 1.80                     | 0.62              |
| 2:CF:19:GLU:HA  | 2:CF:22:ALA:HB3  | 1.82                     | 0.62              |
| 2:GG:19:GLU:HA  | 2:GG:22:ALA:HB3  | 1.82                     | 0.62              |
| 3:PC:105:ILE:HA | 3:PC:179:TYR:HA  | 1.80                     | 0.62              |
| 2:YD:155:HIS:CB | 2:EE:217:ALA:HB2 | 2.29                     | 0.62              |
| 3:ZD:90:HIS:N   | 3:ZD:195:PRO:O   | 2.31                     | 0.62              |
| 3:RE:106:HIS:N  | 3:RE:178:GLU:O   | 2.32                     | 0.62              |
| 2:AG:219:ARG:HA | 2:AG:226:ALA:CB  | 2.29                     | 0.62              |
| 3:FE:90:HIS:N   | 3:FE:195:PRO:O   | 2.31                     | 0.62              |
| 3:RE:90:HIS:N   | 3:RE:195:PRO:O   | 2.31                     | 0.62              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:AG:19:GLU:HA  | 2:AG:22:ALA:HB3 | 1.82                     | 0.62              |
| 2:MG:19:GLU:HA  | 2:MG:22:ALA:HB3 | 1.82                     | 0.62              |
| 3:C:106:HIS:N   | 3:C:178:GLU:O   | 2.32                     | 0.62              |
| 2:J:219:ARG:HA  | 2:J:226:ALA:CB  | 2.29                     | 0.62              |
| 3:BA:106:HIS:N  | 3:BA:178:GLU:O  | 2.32                     | 0.62              |
| 3:HA:106:HIS:N  | 3:HA:178:GLU:O  | 2.32                     | 0.62              |
| 2:EB:19:GLU:HA  | 2:EB:22:ALA:HB3 | 1.82                     | 0.62              |
| 2:KB:19:GLU:HA  | 2:KB:22:ALA:HB3 | 1.82                     | 0.62              |
| 2:QB:219:ARG:HA | 2:QB:226:ALA:CB | 2.29                     | 0.62              |
| 3:JC:106:HIS:N  | 3:JC:178:GLU:O  | 2.32                     | 0.62              |
| 2:QE:19:GLU:HA  | 2:QE:22:ALA:HB3 | 1.82                     | 0.62              |
| 3:JF:106:HIS:N  | 3:JF:178:GLU:O  | 2.32                     | 0.62              |
| 3:M:106:HIS:N   | 3:M:178:GLU:O   | 2.32                     | 0.61              |
| 2:J:19:GLU:HA   | 2:J:22:ALA:HB3  | 1.82                     | 0.61              |
| 2:J:77:LEU:CB   | 2:T:42:ALA:O    | 2.48                     | 0.61              |
| 3:LB:106:HIS:N  | 3:LB:178:GLU:O  | 2.32                     | 0.61              |
| 2:CC:219:ARG:HA | 2:CC:226:ALA:CB | 2.29                     | 0.61              |
| 2:SD:19:GLU:HA  | 2:SD:22:ALA:HB3 | 1.82                     | 0.61              |
| 3:ZD:106:HIS:N  | 3:ZD:178:GLU:O  | 2.32                     | 0.61              |
| 3:DF:90:HIS:N   | 3:DF:195:PRO:O  | 2.31                     | 0.61              |
| 2:GG:219:ARG:HA | 2:GG:226:ALA:CB | 2.29                     | 0.61              |
| 2:B:219:ARG:HA  | 2:B:226:ALA:CB  | 2.29                     | 0.61              |
| 2:MA:219:ARG:HA | 2:MA:226:ALA:CB | 2.29                     | 0.61              |
| 2:SA:219:ARG:HA | 2:SA:226:ALA:CB | 2.29                     | 0.61              |
| 2:YA:219:ARG:HA | 2:YA:226:ALA:CB | 2.29                     | 0.61              |
| 2:OC:19:GLU:HA  | 2:OC:22:ALA:HB3 | 1.82                     | 0.61              |
| 3:VF:106:HIS:N  | 3:VF:178:GLU:O  | 2.32                     | 0.61              |
| 3:C:90:HIS:N    | 3:C:195:PRO:O   | 2.31                     | 0.61              |
| 2:T:219:ARG:HA  | 2:T:226:ALA:CB  | 2.29                     | 0.61              |
| 2:AA:219:ARG:HA | 2:AA:226:ALA:CB | 2.29                     | 0.61              |
| 2:GA:19:GLU:HA  | 2:GA:22:ALA:HB3 | 1.82                     | 0.61              |
| 3:NA:90:HIS:N   | 3:NA:195:PRO:O  | 2.31                     | 0.61              |
| 2:IC:19:GLU:HA  | 2:IC:22:ALA:HB3 | 1.82                     | 0.61              |
| 2:IC:77:LEU:CB  | 2:OC:42:ALA:O   | 2.47                     | 0.61              |
| 3:PC:106:HIS:N  | 3:PC:178:GLU:O  | 2.32                     | 0.61              |
| 2:MD:19:GLU:HA  | 2:MD:22:ALA:HB3 | 1.82                     | 0.61              |
| 2:YD:19:GLU:HA  | 2:YD:22:ALA:HB3 | 1.82                     | 0.61              |
| 3:XE:106:HIS:N  | 3:XE:178:GLU:O  | 2.32                     | 0.61              |
| 2:IF:19:GLU:HA  | 2:IF:22:ALA:HB3 | 1.82                     | 0.61              |
| 2:MG:219:ARG:HA | 2:MG:226:ALA:CB | 2.29                     | 0.61              |
| 2:SG:19:GLU:HA  | 2:SG:22:ALA:HB3 | 1.82                     | 0.61              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:V:90:HIS:N    | 3:V:195:PRO:O    | 2.31                     | 0.61              |
| 2:SA:155:HIS:CB | 2:YA:217:ALA:HB2 | 2.28                     | 0.61              |
| 2:EB:219:ARG:HA | 2:EB:226:ALA:CB  | 2.29                     | 0.61              |
| 3:HD:105:ILE:HA | 3:HD:179:TYR:HA  | 1.80                     | 0.61              |
| 3:TD:90:HIS:N   | 3:TD:195:PRO:O   | 2.31                     | 0.61              |
| 3:TD:105:ILE:HA | 3:TD:179:TYR:HA  | 1.80                     | 0.61              |
| 2:KE:77:LEU:CB  | 2:QE:42:ALA:O    | 2.48                     | 0.61              |
| 3:BG:106:HIS:N  | 3:BG:178:GLU:O   | 2.32                     | 0.61              |
| 2:MA:74:ASN:CA  | 2:SA:42:ALA:O    | 2.48                     | 0.61              |
| 3:FB:106:HIS:N  | 3:FB:178:GLU:O   | 2.32                     | 0.61              |
| 3:XB:106:HIS:N  | 3:XB:178:GLU:O   | 2.32                     | 0.61              |
| 2:YD:68:ALA:HB1 | 2:EE:47:ILE:O    | 2.00                     | 0.61              |
| 2:QE:155:HIS:CB | 2:WE:217:ALA:HB2 | 2.28                     | 0.61              |
| 2:OF:68:ALA:HB1 | 2:UF:47:ILE:O    | 2.00                     | 0.61              |
| 2:SG:219:ARG:HA | 2:SG:226:ALA:CB  | 2.29                     | 0.61              |
| 2:G:219:ARG:HA  | 2:G:226:ALA:CB   | 2.29                     | 0.61              |
| 3:HA:90:HIS:N   | 3:HA:195:PRO:O   | 2.31                     | 0.61              |
| 3:ZA:106:HIS:N  | 3:ZA:178:GLU:O   | 2.32                     | 0.61              |
| 2:KB:219:ARG:HA | 2:KB:226:ALA:CB  | 2.29                     | 0.61              |
| 2:CC:155:HIS:CB | 2:IC:217:ALA:HB2 | 2.30                     | 0.61              |
| 3:HD:106:HIS:N  | 3:HD:178:GLU:O   | 2.32                     | 0.61              |
| 3:ND:90:HIS:N   | 3:ND:195:PRO:O   | 2.31                     | 0.61              |
| 3:K:106:HIS:N   | 3:K:178:GLU:O    | 2.32                     | 0.61              |
| 3:V:106:HIS:N   | 3:V:178:GLU:O    | 2.32                     | 0.61              |
| 3:NA:106:HIS:N  | 3:NA:178:GLU:O   | 2.32                     | 0.61              |
| 2:CC:19:GLU:HA  | 2:CC:22:ALA:HB3  | 1.82                     | 0.61              |
| 2:SD:155:HIS:CB | 2:YD:217:ALA:HB2 | 2.29                     | 0.61              |
| 2:UF:19:GLU:HA  | 2:UF:22:ALA:HB3  | 1.82                     | 0.61              |
| 3:NG:106:HIS:N  | 3:NG:178:GLU:O   | 2.32                     | 0.61              |
| 3:TG:90:HIS:N   | 3:TG:195:PRO:O   | 2.31                     | 0.61              |
| 3:TG:106:HIS:N  | 3:TG:178:GLU:O   | 2.32                     | 0.61              |
| 2:B:19:GLU:HA   | 2:B:22:ALA:HB3   | 1.82                     | 0.61              |
| 2:SA:19:GLU:HA  | 2:SA:22:ALA:HB3  | 1.82                     | 0.61              |
| 3:TA:106:HIS:N  | 3:TA:178:GLU:O   | 2.32                     | 0.61              |
| 3:RB:106:HIS:N  | 3:RB:178:GLU:O   | 2.32                     | 0.61              |
| 2:WB:219:ARG:HA | 2:WB:226:ALA:CB  | 2.29                     | 0.61              |
| 2:UC:19:GLU:HA  | 2:UC:22:ALA:HB3  | 1.82                     | 0.61              |
| 3:HG:106:HIS:N  | 3:HG:178:GLU:O   | 2.32                     | 0.61              |
| 3:ZA:90:HIS:N   | 3:ZA:195:PRO:O   | 2.31                     | 0.61              |
| 2:QB:19:GLU:HA  | 2:QB:22:ALA:HB3  | 1.82                     | 0.61              |
| 3:HD:90:HIS:N   | 3:HD:195:PRO:O   | 2.31                     | 0.61              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:WE:68:ALA:HB1 | 2:CF:47:ILE:O    | 2.00                     | 0.61              |
| 4:OA:97:LEU:N   | 4:OA:109:GLY:O   | 2.34                     | 0.61              |
| 4:AB:97:LEU:N   | 4:AB:109:GLY:O   | 2.34                     | 0.61              |
| 4:GB:97:LEU:N   | 4:GB:109:GLY:O   | 2.34                     | 0.61              |
| 2:GD:19:GLU:HA  | 2:GD:22:ALA:HB3  | 1.82                     | 0.61              |
| 2:MD:68:ALA:HB1 | 2:SD:47:ILE:O    | 2.00                     | 0.61              |
| 2:WE:74:ASN:CA  | 2:CF:42:ALA:O    | 2.48                     | 0.61              |
| 2:GG:68:ALA:HB1 | 2:MG:47:ILE:O    | 2.00                     | 0.61              |
| 4:CA:97:LEU:N   | 4:CA:109:GLY:O   | 2.34                     | 0.60              |
| 4:IA:97:LEU:N   | 4:IA:109:GLY:O   | 2.34                     | 0.60              |
| 4:UA:97:LEU:N   | 4:UA:109:GLY:O   | 2.34                     | 0.60              |
| 2:EE:19:GLU:HA  | 2:EE:22:ALA:HB3  | 1.82                     | 0.60              |
| 3:PF:106:HIS:N  | 3:PF:178:GLU:O   | 2.32                     | 0.60              |
| 2:GG:155:HIS:CB | 2:MG:217:ALA:HB2 | 2.29                     | 0.60              |
| 2:G:19:GLU:HA   | 2:G:22:ALA:HB3   | 1.82                     | 0.60              |
| 3:TA:90:HIS:N   | 3:TA:195:PRO:O   | 2.31                     | 0.60              |
| 4:MB:97:LEU:N   | 4:MB:109:GLY:O   | 2.34                     | 0.60              |
| 3:VC:90:HIS:N   | 3:VC:195:PRO:O   | 2.31                     | 0.60              |
| 2:OF:19:GLU:HA  | 2:OF:22:ALA:HB3  | 1.82                     | 0.60              |
| 4:L:97:LEU:N    | 4:L:109:GLY:O    | 2.34                     | 0.60              |
| 2:MA:19:GLU:HA  | 2:MA:22:ALA:HB3  | 1.82                     | 0.60              |
| 3:LB:90:HIS:N   | 3:LB:195:PRO:O   | 2.31                     | 0.60              |
| 4:SB:97:LEU:N   | 4:SB:109:GLY:O   | 2.34                     | 0.60              |
| 3:BD:90:HIS:N   | 3:BD:195:PRO:O   | 2.31                     | 0.60              |
| 2:KE:19:GLU:HA  | 2:KE:22:ALA:HB3  | 1.82                     | 0.60              |
| 4:W:97:LEU:N    | 4:W:109:GLY:O    | 2.34                     | 0.60              |
| 2:QB:155:HIS:CB | 2:WB:217:ALA:HB2 | 2.31                     | 0.60              |
| 2:WB:77:LEU:CB  | 2:CC:42:ALA:O    | 2.49                     | 0.60              |
| 2:AD:68:ALA:HB1 | 2:GD:47:ILE:O    | 2.01                     | 0.60              |
| 4:SE:97:LEU:N   | 4:SE:109:GLY:O   | 2.34                     | 0.60              |
| 2:G:42:ALA:O    | 2:SG:77:LEU:CB   | 2.49                     | 0.60              |
| 2:T:68:ALA:HB1  | 2:AA:47:ILE:O    | 2.02                     | 0.60              |
| 3:FB:90:HIS:N   | 3:FB:195:PRO:O   | 2.31                     | 0.60              |
| 4:YB:97:LEU:N   | 4:YB:109:GLY:O   | 2.34                     | 0.60              |
| 3:JC:90:HIS:N   | 3:JC:195:PRO:O   | 2.31                     | 0.60              |
| 4:GE:97:LEU:N   | 4:GE:109:GLY:O   | 2.34                     | 0.60              |
| 4:ME:97:LEU:N   | 4:ME:109:GLY:O   | 2.34                     | 0.60              |
| 3:HG:90:HIS:N   | 3:HG:195:PRO:O   | 2.31                     | 0.60              |
| 3:XB:90:HIS:N   | 3:XB:195:PRO:O   | 2.31                     | 0.60              |
| 4:YE:97:LEU:N   | 4:YE:109:GLY:O   | 2.34                     | 0.60              |
| 2:OF:74:ASN:CA  | 2:UF:42:ALA:O    | 2.49                     | 0.60              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:D:97:LEU:N    | 4:D:109:GLY:O    | 2.34                     | 0.60              |
| 3:PC:90:HIS:N   | 3:PC:195:PRO:O   | 2.31                     | 0.60              |
| 3:V:314:ALA:HA  | 4:W:88:ALA:HA    | 1.84                     | 0.60              |
| 2:AA:77:LEU:CB  | 2:GA:42:ALA:O    | 2.49                     | 0.60              |
| 3:ZA:314:ALA:HA | 4:AB:88:ALA:HA   | 1.84                     | 0.60              |
| 3:FB:314:ALA:HA | 4:GB:88:ALA:HA   | 1.84                     | 0.60              |
| 2:WB:19:GLU:HA  | 2:WB:22:ALA:HB3  | 1.82                     | 0.60              |
| 3:DC:314:ALA:HA | 4:EC:88:ALA:HA   | 1.84                     | 0.60              |
| 4:EC:97:LEU:N   | 4:EC:109:GLY:O   | 2.34                     | 0.60              |
| 2:MD:155:HIS:CB | 2:SD:217:ALA:HB2 | 2.31                     | 0.60              |
| 2:SD:77:LEU:CB  | 2:YD:42:ALA:O    | 2.50                     | 0.60              |
| 4:AE:97:LEU:N   | 4:AE:109:GLY:O   | 2.34                     | 0.60              |
| 4:EF:97:LEU:N   | 4:EF:109:GLY:O   | 2.34                     | 0.60              |
| 4:N:97:LEU:N    | 4:N:109:GLY:O    | 2.34                     | 0.60              |
| 2:T:74:ASN:CA   | 2:AA:42:ALA:O    | 2.50                     | 0.60              |
| 3:RB:90:HIS:N   | 3:RB:195:PRO:O   | 2.31                     | 0.60              |
| 3:JC:314:ALA:HA | 4:KC:88:ALA:HA   | 1.84                     | 0.60              |
| 4:KF:97:LEU:N   | 4:KF:109:GLY:O   | 2.34                     | 0.60              |
| 2:AG:68:ALA:HB1 | 2:GG:47:ILE:O    | 2.02                     | 0.60              |
| 2:G:155:HIS:CB  | 2:B:217:ALA:HB2  | 2.30                     | 0.60              |
| 3:K:314:ALA:HA  | 4:L:88:ALA:HA    | 1.84                     | 0.60              |
| 3:BA:314:ALA:HA | 4:CA:88:ALA:HA   | 1.84                     | 0.60              |
| 3:DC:90:HIS:N   | 3:DC:195:PRO:O   | 2.31                     | 0.60              |
| 2:AD:19:GLU:HA  | 2:AD:22:ALA:HB3  | 1.82                     | 0.60              |
| 3:ND:314:ALA:HA | 4:OD:88:ALA:HA   | 1.84                     | 0.60              |
| 4:UD:97:LEU:N   | 4:UD:109:GLY:O   | 2.34                     | 0.60              |
| 2:EE:77:LEU:CB  | 2:KE:42:ALA:O    | 2.50                     | 0.60              |
| 2:GA:74:ASN:CA  | 2:MA:42:ALA:O    | 2.50                     | 0.59              |
| 2:GA:77:LEU:CB  | 2:MA:42:ALA:O    | 2.50                     | 0.59              |
| 2:EB:77:LEU:CB  | 2:KB:42:ALA:O    | 2.50                     | 0.59              |
| 4:KC:97:LEU:N   | 4:KC:109:GLY:O   | 2.34                     | 0.59              |
| 3:HD:314:ALA:HA | 4:ID:88:ALA:HA   | 1.84                     | 0.59              |
| 3:ND:102:LEU:O  | 3:ND:183:GLU:N   | 2.31                     | 0.59              |
| 3:TD:314:ALA:HA | 4:UD:88:ALA:HA   | 1.84                     | 0.59              |
| 3:PC:314:ALA:HA | 4:QC:88:ALA:HA   | 1.84                     | 0.59              |
| 4:DD:122:ILE:O  | 4:ED:84:GLY:N    | 2.34                     | 0.59              |
| 4:PD:122:ILE:O  | 4:QD:84:GLY:N    | 2.34                     | 0.59              |
| 4:HE:122:ILE:O  | 4:IE:84:GLY:N    | 2.34                     | 0.59              |
| 4:UG:97:LEU:N   | 4:UG:109:GLY:O   | 2.34                     | 0.59              |
| 3:TA:314:ALA:HA | 4:UA:88:ALA:HA   | 1.84                     | 0.59              |
| 4:NB:122:ILE:O  | 4:OB:84:GLY:N    | 2.34                     | 0.59              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:XB:314:ALA:HA | 4:YB:88:ALA:HA   | 1.84                     | 0.59              |
| 2:AD:77:LEU:CB  | 2:GD:42:ALA:O    | 2.50                     | 0.59              |
| 4:JD:122:ILE:O  | 4:KD:84:GLY:N    | 2.34                     | 0.59              |
| 4:VD:122:ILE:O  | 4:WD:84:GLY:N    | 2.34                     | 0.59              |
| 4:BE:122:ILE:O  | 4:CE:84:GLY:N    | 2.34                     | 0.59              |
| 4:QF:97:LEU:N   | 4:QF:109:GLY:O   | 2.34                     | 0.59              |
| 2:UF:155:HIS:CB | 2:AG:217:ALA:HB2 | 2.29                     | 0.59              |
| 2:GG:74:ASN:CA  | 2:MG:42:ALA:O    | 2.49                     | 0.59              |
| 2:B:77:LEU:CB   | 2:J:42:ALA:O     | 2.50                     | 0.59              |
| 4:HB:122:ILE:O  | 4:IB:84:GLY:N    | 2.34                     | 0.59              |
| 4:OD:97:LEU:N   | 4:OD:109:GLY:O   | 2.34                     | 0.59              |
| 4:NE:122:ILE:O  | 4:OE:84:GLY:N    | 2.34                     | 0.59              |
| 4:TE:122:ILE:O  | 4:UE:84:GLY:N    | 2.34                     | 0.59              |
| 2:GA:68:ALA:HB1 | 2:MA:47:ILE:O    | 2.01                     | 0.59              |
| 2:SA:77:LEU:CB  | 2:YA:42:ALA:O    | 2.50                     | 0.59              |
| 3:LB:314:ALA:HA | 4:MB:88:ALA:HA   | 1.84                     | 0.59              |
| 3:HD:102:LEU:O  | 3:HD:183:GLU:N   | 2.31                     | 0.59              |
| 3:RE:314:ALA:HA | 4:SE:88:ALA:HA   | 1.84                     | 0.59              |
| 4:ZE:122:ILE:O  | 4:AF:84:GLY:N    | 2.34                     | 0.59              |
| 4:FF:122:ILE:O  | 4:GF:84:GLY:N    | 2.34                     | 0.59              |
| 2:UF:68:ALA:HB1 | 2:AG:47:ILE:O    | 2.02                     | 0.59              |
| 3:HG:314:ALA:HA | 4:IG:88:ALA:HA   | 1.84                     | 0.59              |
| 4:VA:122:ILE:O  | 4:WA:84:GLY:N    | 2.34                     | 0.59              |
| 4:BB:122:ILE:O  | 4:CB:84:GLY:N    | 2.34                     | 0.59              |
| 2:UC:155:HIS:CB | 2:AD:217:ALA:HB2 | 2.32                     | 0.59              |
| 2:QE:68:ALA:HB1 | 2:WE:47:ILE:O    | 2.02                     | 0.59              |
| 3:XE:314:ALA:HA | 4:YE:88:ALA:HA   | 1.84                     | 0.59              |
| 3:NG:314:ALA:HA | 4:OG:88:ALA:HA   | 1.84                     | 0.59              |
| 4:OG:97:LEU:N   | 4:OG:109:GLY:O   | 2.34                     | 0.59              |
| 2:KB:155:HIS:CB | 2:QB:217:ALA:HB2 | 2.27                     | 0.59              |
| 2:EE:155:HIS:CB | 2:KE:217:ALA:HB2 | 2.30                     | 0.59              |
| 4:LF:122:ILE:O  | 4:MF:84:GLY:N    | 2.34                     | 0.59              |
| 3:VF:90:HIS:N   | 3:VF:195:PRO:O   | 2.31                     | 0.59              |
| 3:BG:314:ALA:HA | 4:CG:88:ALA:HA   | 1.84                     | 0.59              |
| 2:G:68:ALA:HB1  | 2:B:47:ILE:O     | 2.03                     | 0.59              |
| 3:C:102:LEU:O   | 3:C:183:GLU:N    | 2.31                     | 0.59              |
| 3:C:314:ALA:HA  | 4:D:88:ALA:HA    | 1.84                     | 0.59              |
| 3:HA:314:ALA:HA | 4:IA:88:ALA:HA   | 1.84                     | 0.59              |
| 3:BD:314:ALA:HA | 4:CD:88:ALA:HA   | 1.84                     | 0.59              |
| 3:DF:314:ALA:HA | 4:EF:88:ALA:HA   | 1.84                     | 0.59              |
| 4:IG:97:LEU:N   | 4:IG:109:GLY:O   | 2.34                     | 0.59              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 3:TG:102:LEU:O  | 3:TG:183:GLU:N | 2.31                     | 0.59              |
| 3:M:102:LEU:O   | 3:M:183:GLU:N  | 2.31                     | 0.59              |
| 2:B:68:ALA:HB1  | 2:J:47:ILE:O   | 2.03                     | 0.59              |
| 3:K:102:LEU:O   | 3:K:183:GLU:N  | 2.31                     | 0.59              |
| 4:O:97:LEU:N    | 4:O:109:GLY:O  | 2.36                     | 0.59              |
| 4:JA:122:ILE:O  | 4:KA:84:GLY:N  | 2.34                     | 0.59              |
| 4:PA:122:ILE:O  | 4:QA:84:GLY:N  | 2.34                     | 0.59              |
| 2:AD:74:ASN:CA  | 2:GD:42:ALA:O  | 2.50                     | 0.59              |
| 4:ID:97:LEU:N   | 4:ID:109:GLY:O | 2.34                     | 0.59              |
| 4:RF:122:ILE:O  | 4:SF:84:GLY:N  | 2.34                     | 0.59              |
| 4:WF:97:LEU:N   | 4:WF:109:GLY:O | 2.34                     | 0.59              |
| 2:G:74:ASN:CA   | 2:B:42:ALA:O   | 2.51                     | 0.59              |
| 4:E:97:LEU:N    | 4:E:109:GLY:O  | 2.36                     | 0.59              |
| 3:V:102:LEU:O   | 3:V:183:GLU:N  | 2.31                     | 0.59              |
| 4:X:97:LEU:N    | 4:X:109:GLY:O  | 2.36                     | 0.59              |
| 2:EB:68:ALA:HB1 | 2:KB:47:ILE:O  | 2.03                     | 0.59              |
| 3:BD:102:LEU:O  | 3:BD:183:GLU:N | 2.31                     | 0.59              |
| 2:GD:77:LEU:CB  | 2:MD:42:ALA:O  | 2.51                     | 0.59              |
| 3:ZD:314:ALA:HA | 4:AE:88:ALA:HA | 1.84                     | 0.59              |
| 4:NE:97:LEU:N   | 4:NE:109:GLY:O | 2.36                     | 0.59              |
| 4:TE:97:LEU:N   | 4:TE:109:GLY:O | 2.36                     | 0.59              |
| 4:ZE:97:LEU:N   | 4:ZE:109:GLY:O | 2.36                     | 0.59              |
| 4:FF:97:LEU:N   | 4:FF:109:GLY:O | 2.36                     | 0.59              |
| 4:RF:97:LEU:N   | 4:RF:109:GLY:O | 2.36                     | 0.59              |
| 4:XF:97:LEU:N   | 4:XF:109:GLY:O | 2.36                     | 0.59              |
| 4:XF:122:ILE:O  | 4:YF:84:GLY:N  | 2.34                     | 0.59              |
| 3:TG:314:ALA:HA | 4:UG:88:ALA:HA | 1.84                     | 0.59              |
| 4:VG:97:LEU:N   | 4:VG:109:GLY:O | 2.36                     | 0.59              |
| 4:P:97:LEU:N    | 4:P:109:GLY:O  | 2.36                     | 0.58              |
| 2:T:77:LEU:CB   | 2:AA:42:ALA:O  | 2.51                     | 0.58              |
| 4:DA:97:LEU:N   | 4:DA:109:GLY:O | 2.36                     | 0.58              |
| 4:DA:122:ILE:O  | 4:EA:84:GLY:N  | 2.34                     | 0.58              |
| 4:JA:97:LEU:N   | 4:JA:109:GLY:O | 2.36                     | 0.58              |
| 4:PA:97:LEU:N   | 4:PA:109:GLY:O | 2.36                     | 0.58              |
| 2:MD:74:ASN:CA  | 2:SD:42:ALA:O  | 2.49                     | 0.58              |
| 4:HE:97:LEU:N   | 4:HE:109:GLY:O | 2.36                     | 0.58              |
| 2:CF:77:LEU:CB  | 2:IF:42:ALA:O  | 2.51                     | 0.58              |
| 4:LF:97:LEU:N   | 4:LF:109:GLY:O | 2.36                     | 0.58              |
| 2:AG:74:ASN:CA  | 2:GG:42:ALA:O  | 2.50                     | 0.58              |
| 4:DG:122:ILE:O  | 4:EG:84:GLY:N  | 2.34                     | 0.58              |
| 4:JG:97:LEU:N   | 4:JG:109:GLY:O | 2.36                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:PG:97:LEU:N   | 4:PG:109:GLY:O   | 2.36                     | 0.58              |
| 4:X:122:ILE:O   | 4:Y:84:GLY:N     | 2.34                     | 0.58              |
| 3:VC:314:ALA:HA | 4:WC:88:ALA:HA   | 1.84                     | 0.58              |
| 4:BE:97:LEU:N   | 4:BE:109:GLY:O   | 2.36                     | 0.58              |
| 3:LE:314:ALA:HA | 4:ME:88:ALA:HA   | 1.84                     | 0.58              |
| 4:DG:97:LEU:N   | 4:DG:109:GLY:O   | 2.36                     | 0.58              |
| 4:JG:122:ILE:O  | 4:KG:84:GLY:N    | 2.34                     | 0.58              |
| 2:MG:155:HIS:CB | 2:SG:217:ALA:HB2 | 2.31                     | 0.58              |
| 4:PG:122:ILE:O  | 4:QG:84:GLY:N    | 2.34                     | 0.58              |
| 4:E:122:ILE:O   | 4:H:84:GLY:N     | 2.34                     | 0.58              |
| 4:O:122:ILE:O   | 4:R:84:GLY:N     | 2.34                     | 0.58              |
| 3:BA:102:LEU:O  | 3:BA:183:GLU:N   | 2.31                     | 0.58              |
| 3:NA:314:ALA:HA | 4:OA:88:ALA:HA   | 1.84                     | 0.58              |
| 4:VA:97:LEU:N   | 4:VA:109:GLY:O   | 2.36                     | 0.58              |
| 4:PD:97:LEU:N   | 4:PD:109:GLY:O   | 2.36                     | 0.58              |
| 4:VD:97:LEU:N   | 4:VD:109:GLY:O   | 2.36                     | 0.58              |
| 2:CF:155:HIS:CB | 2:IF:217:ALA:HB2 | 2.28                     | 0.58              |
| 4:CG:97:LEU:N   | 4:CG:109:GLY:O   | 2.34                     | 0.58              |
| 4:P:122:ILE:O   | 4:Q:84:GLY:N     | 2.34                     | 0.58              |
| 2:B:74:ASN:CA   | 2:J:42:ALA:O     | 2.52                     | 0.58              |
| 3:VC:102:LEU:O  | 3:VC:183:GLU:N   | 2.31                     | 0.58              |
| 4:JD:97:LEU:N   | 4:JD:109:GLY:O   | 2.36                     | 0.58              |
| 3:JF:314:ALA:HA | 4:KF:88:ALA:HA   | 1.84                     | 0.58              |
| 3:VF:314:ALA:HA | 4:WF:88:ALA:HA   | 1.84                     | 0.58              |
| 4:VG:122:ILE:O  | 4:WG:84:GLY:N    | 2.34                     | 0.58              |
| 4:BB:97:LEU:N   | 4:BB:109:GLY:O   | 2.37                     | 0.58              |
| 4:HB:97:LEU:N   | 4:HB:109:GLY:O   | 2.36                     | 0.58              |
| 2:KE:68:ALA:HB1 | 2:QE:47:ILE:O    | 2.03                     | 0.58              |
| 3:HA:102:LEU:O  | 3:HA:183:GLU:N   | 2.31                     | 0.58              |
| 4:NB:97:LEU:N   | 4:NB:109:GLY:O   | 2.36                     | 0.58              |
| 4:AC:65:THR:N   | 4:AC:100:LEU:O   | 2.37                     | 0.58              |
| 4:LC:97:LEU:N   | 4:LC:109:GLY:O   | 2.36                     | 0.58              |
| 4:QC:97:LEU:N   | 4:QC:109:GLY:O   | 2.34                     | 0.58              |
| 4:RC:97:LEU:N   | 4:RC:109:GLY:O   | 2.36                     | 0.58              |
| 2:UC:68:ALA:HB1 | 2:AD:47:ILE:O    | 2.03                     | 0.58              |
| 4:WC:97:LEU:N   | 4:WC:109:GLY:O   | 2.34                     | 0.58              |
| 4:XC:97:LEU:N   | 4:XC:109:GLY:O   | 2.36                     | 0.58              |
| 4:DD:97:LEU:N   | 4:DD:109:GLY:O   | 2.36                     | 0.58              |
| 2:MG:77:LEU:CB  | 2:SG:42:ALA:O    | 2.50                     | 0.58              |
| 3:RB:314:ALA:HA | 4:SB:88:ALA:HA   | 1.84                     | 0.58              |
| 4:TB:97:LEU:N   | 4:TB:109:GLY:O   | 2.36                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:CD:97:LEU:N   | 4:CD:109:GLY:O   | 2.34                     | 0.58              |
| 2:GD:68:ALA:HB1 | 2:MD:47:ILE:O    | 2.03                     | 0.58              |
| 2:QE:77:LEU:CB  | 2:WE:42:ALA:O    | 2.51                     | 0.58              |
| 2:UF:74:ASN:CA  | 2:AG:42:ALA:O    | 2.51                     | 0.58              |
| 2:AG:77:LEU:CB  | 2:GG:42:ALA:O    | 2.51                     | 0.58              |
| 3:M:314:ALA:HA  | 4:N:88:ALA:HA    | 1.84                     | 0.58              |
| 2:QB:77:LEU:CB  | 2:WB:42:ALA:O    | 2.51                     | 0.58              |
| 4:ZB:97:LEU:N   | 4:ZB:109:GLY:O   | 2.36                     | 0.58              |
| 4:FC:97:LEU:N   | 4:FC:109:GLY:O   | 2.36                     | 0.58              |
| 3:PC:102:LEU:O  | 3:PC:183:GLU:N   | 2.31                     | 0.58              |
| 2:QE:74:ASN:CA  | 2:WE:42:ALA:O    | 2.50                     | 0.58              |
| 3:NA:102:LEU:O  | 3:NA:183:GLU:N   | 2.31                     | 0.58              |
| 2:OF:77:LEU:CB  | 2:UF:42:ALA:O    | 2.52                     | 0.58              |
| 2:CC:77:LEU:CB  | 2:IC:42:ALA:O    | 2.51                     | 0.58              |
| 4:GC:65:THR:N   | 4:GC:100:LEU:O   | 2.37                     | 0.58              |
| 3:FE:314:ALA:HA | 4:GE:88:ALA:HA   | 1.84                     | 0.58              |
| 2:WE:155:HIS:CB | 2:CF:217:ALA:HB2 | 2.31                     | 0.58              |
| 3:VF:102:LEU:O  | 3:VF:183:GLU:N   | 2.31                     | 0.58              |
| 4:R:65:THR:N    | 4:R:100:LEU:O    | 2.37                     | 0.57              |
| 4:Y:65:THR:N    | 4:Y:100:LEU:O    | 2.37                     | 0.57              |
| 4:EA:65:THR:N   | 4:EA:100:LEU:O   | 2.37                     | 0.57              |
| 4:QA:65:THR:N   | 4:QA:100:LEU:O   | 2.37                     | 0.57              |
| 2:SA:68:ALA:HB1 | 2:YA:47:ILE:O    | 2.04                     | 0.57              |
| 3:TA:102:LEU:O  | 3:TA:183:GLU:N   | 2.31                     | 0.57              |
| 4:WA:65:THR:N   | 4:WA:100:LEU:O   | 2.37                     | 0.57              |
| 4:CB:65:THR:N   | 4:CB:100:LEU:O   | 2.37                     | 0.57              |
| 4:IB:65:THR:N   | 4:IB:100:LEU:O   | 2.37                     | 0.57              |
| 3:TD:88:PRO:HA  | 3:TD:198:ILE:HA  | 1.86                     | 0.57              |
| 2:UF:77:LEU:CB  | 2:AG:42:ALA:O    | 2.52                     | 0.57              |
| 4:EG:65:THR:N   | 4:EG:100:LEU:O   | 2.37                     | 0.57              |
| 2:G:47:ILE:O    | 2:SG:68:ALA:HB1  | 2.03                     | 0.57              |
| 4:Q:65:THR:N    | 4:Q:100:LEU:O    | 2.37                     | 0.57              |
| 4:H:65:THR:N    | 4:H:100:LEU:O    | 2.37                     | 0.57              |
| 4:KA:65:THR:N   | 4:KA:100:LEU:O   | 2.37                     | 0.57              |
| 4:OB:65:THR:N   | 4:OB:100:LEU:O   | 2.37                     | 0.57              |
| 4:UB:65:THR:N   | 4:UB:100:LEU:O   | 2.37                     | 0.57              |
| 3:JC:102:LEU:O  | 3:JC:183:GLU:N   | 2.31                     | 0.57              |
| 2:OC:77:LEU:CB  | 2:UC:42:ALA:O    | 2.52                     | 0.57              |
| 2:YD:74:ASN:CA  | 2:EE:42:ALA:O    | 2.49                     | 0.57              |
| 3:FE:88:PRO:HA  | 3:FE:198:ILE:HA  | 1.86                     | 0.57              |
| 2:CF:68:ALA:HB1 | 2:IF:47:ILE:O    | 2.03                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:WG:65:THR:N   | 4:WG:100:LEU:O  | 2.37                     | 0.57              |
| 3:ZA:102:LEU:O  | 3:ZA:183:GLU:N  | 2.31                     | 0.57              |
| 2:WB:74:ASN:CA  | 2:CC:42:ALA:O   | 2.53                     | 0.57              |
| 3:XB:85:ARG:N   | 3:XB:201:ASN:O  | 2.36                     | 0.57              |
| 2:UC:77:LEU:CB  | 2:AD:42:ALA:O   | 2.52                     | 0.57              |
| 3:HD:88:PRO:HA  | 3:HD:198:ILE:HA | 1.86                     | 0.57              |
| 3:LE:88:PRO:HA  | 3:LE:198:ILE:HA | 1.86                     | 0.57              |
| 3:PF:314:ALA:HA | 4:QF:88:ALA:HA  | 1.84                     | 0.57              |
| 4:QG:65:THR:N   | 4:QG:100:LEU:O  | 2.37                     | 0.57              |
| 2:G:77:LEU:CB   | 2:B:42:ALA:O    | 2.52                     | 0.57              |
| 2:CC:68:ALA:HB1 | 2:IC:47:ILE:O   | 2.04                     | 0.57              |
| 2:CC:74:ASN:CA  | 2:IC:42:ALA:O   | 2.53                     | 0.57              |
| 3:DC:102:LEU:O  | 3:DC:183:GLU:N  | 2.31                     | 0.57              |
| 4:KG:65:THR:N   | 4:KG:100:LEU:O  | 2.37                     | 0.57              |
| 3:K:88:PRO:HA   | 3:K:198:ILE:HA  | 1.86                     | 0.57              |
| 3:HA:88:PRO:HA  | 3:HA:198:ILE:HA | 1.86                     | 0.57              |
| 3:FB:102:LEU:O  | 3:FB:183:GLU:N  | 2.31                     | 0.57              |
| 3:LB:102:LEU:O  | 3:LB:183:GLU:N  | 2.31                     | 0.57              |
| 3:XB:102:LEU:O  | 3:XB:183:GLU:N  | 2.31                     | 0.57              |
| 4:MC:65:THR:N   | 4:MC:100:LEU:O  | 2.37                     | 0.57              |
| 3:VC:88:PRO:HA  | 3:VC:198:ILE:HA | 1.86                     | 0.57              |
| 3:ND:88:PRO:HA  | 3:ND:198:ILE:HA | 1.86                     | 0.57              |
| 2:YD:77:LEU:CB  | 2:EE:42:ALA:O   | 2.52                     | 0.57              |
| 3:FE:85:ARG:N   | 3:FE:201:ASN:O  | 2.36                     | 0.57              |
| 3:XE:88:PRO:HA  | 3:XE:198:ILE:HA | 1.86                     | 0.57              |
| 3:PF:102:LEU:O  | 3:PF:183:GLU:N  | 2.31                     | 0.57              |
| 4:YF:65:THR:N   | 4:YF:100:LEU:O  | 2.37                     | 0.57              |
| 3:NA:88:PRO:HA  | 3:NA:198:ILE:HA | 1.86                     | 0.57              |
| 3:ZA:88:PRO:HA  | 3:ZA:198:ILE:HA | 1.86                     | 0.57              |
| 3:RB:102:LEU:O  | 3:RB:183:GLU:N  | 2.31                     | 0.57              |
| 3:ZD:88:PRO:HA  | 3:ZD:198:ILE:HA | 1.86                     | 0.57              |
| 4:IE:65:THR:N   | 4:IE:100:LEU:O  | 2.37                     | 0.57              |
| 3:V:88:PRO:HA   | 3:V:198:ILE:HA  | 1.86                     | 0.57              |
| 3:RB:85:ARG:N   | 3:RB:201:ASN:O  | 2.36                     | 0.57              |
| 3:BD:88:PRO:HA  | 3:BD:198:ILE:HA | 1.86                     | 0.57              |
| 3:ZD:85:ARG:N   | 3:ZD:201:ASN:O  | 2.36                     | 0.57              |
| 3:LE:85:ARG:N   | 3:LE:201:ASN:O  | 2.36                     | 0.57              |
| 4:OE:65:THR:N   | 4:OE:100:LEU:O  | 2.37                     | 0.57              |
| 3:RE:88:PRO:HA  | 3:RE:198:ILE:HA | 1.86                     | 0.57              |
| 4:AF:65:THR:N   | 4:AF:100:LEU:O  | 2.37                     | 0.57              |
| 3:JF:88:PRO:HA  | 3:JF:198:ILE:HA | 1.86                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:MF:65:THR:N   | 4:MF:100:LEU:O  | 2.37                     | 0.57              |
| 4:SF:65:THR:N   | 4:SF:100:LEU:O  | 2.37                     | 0.57              |
| 3:TG:88:PRO:HA  | 3:TG:198:ILE:HA | 1.86                     | 0.57              |
| 3:PC:88:PRO:HA  | 3:PC:198:ILE:HA | 1.86                     | 0.57              |
| 2:UC:74:ASN:CA  | 2:AD:42:ALA:O   | 2.52                     | 0.57              |
| 2:GD:74:ASN:CA  | 2:MD:42:ALA:O   | 2.51                     | 0.57              |
| 4:CE:65:THR:N   | 4:CE:100:LEU:O  | 2.37                     | 0.57              |
| 4:UE:65:THR:N   | 4:UE:100:LEU:O  | 2.37                     | 0.57              |
| 3:PC:85:ARG:N   | 3:PC:201:ASN:O  | 2.36                     | 0.57              |
| 4:SC:65:THR:N   | 4:SC:100:LEU:O  | 2.37                     | 0.57              |
| 4:WD:65:THR:N   | 4:WD:100:LEU:O  | 2.37                     | 0.57              |
| 3:DF:88:PRO:HA  | 3:DF:198:ILE:HA | 1.86                     | 0.57              |
| 3:M:88:PRO:HA   | 3:M:198:ILE:HA  | 1.86                     | 0.57              |
| 3:RB:201:ASN:HA | 3:RB:218:CYS:HA | 1.87                     | 0.57              |
| 4:YC:65:THR:N   | 4:YC:100:LEU:O  | 2.37                     | 0.57              |
| 3:BD:201:ASN:HA | 3:BD:218:CYS:HA | 1.87                     | 0.57              |
| 3:ND:201:ASN:HA | 3:ND:218:CYS:HA | 1.87                     | 0.57              |
| 4:GF:65:THR:N   | 4:GF:100:LEU:O  | 2.37                     | 0.57              |
| 3:JF:102:LEU:O  | 3:JF:183:GLU:N  | 2.31                     | 0.57              |
| 3:VF:88:PRO:HA  | 3:VF:198:ILE:HA | 1.86                     | 0.57              |
| 3:NA:201:ASN:HA | 3:NA:218:CYS:HA | 1.87                     | 0.56              |
| 3:DC:201:ASN:HA | 3:DC:218:CYS:HA | 1.87                     | 0.56              |
| 3:JC:201:ASN:HA | 3:JC:218:CYS:HA | 1.87                     | 0.56              |
| 4:ED:65:THR:N   | 4:ED:100:LEU:O  | 2.37                     | 0.56              |
| 3:HD:201:ASN:HA | 3:HD:218:CYS:HA | 1.87                     | 0.56              |
| 4:QD:65:THR:N   | 4:QD:100:LEU:O  | 2.37                     | 0.56              |
| 2:AA:74:ASN:CA  | 2:GA:42:ALA:O   | 2.53                     | 0.56              |
| 3:TA:201:ASN:HA | 3:TA:218:CYS:HA | 1.87                     | 0.56              |
| 3:FB:88:PRO:HA  | 3:FB:198:ILE:HA | 1.86                     | 0.56              |
| 3:FB:201:ASN:HA | 3:FB:218:CYS:HA | 1.88                     | 0.56              |
| 3:RB:88:PRO:HA  | 3:RB:198:ILE:HA | 1.86                     | 0.56              |
| 3:XB:201:ASN:HA | 3:XB:218:CYS:HA | 1.87                     | 0.56              |
| 3:JC:88:PRO:HA  | 3:JC:198:ILE:HA | 1.86                     | 0.56              |
| 3:PC:201:ASN:HA | 3:PC:218:CYS:HA | 1.87                     | 0.56              |
| 3:VC:201:ASN:HA | 3:VC:218:CYS:HA | 1.87                     | 0.56              |
| 4:KD:65:THR:N   | 4:KD:100:LEU:O  | 2.37                     | 0.56              |
| 3:TD:201:ASN:HA | 3:TD:218:CYS:HA | 1.87                     | 0.56              |
| 3:LE:201:ASN:HA | 3:LE:218:CYS:HA | 1.87                     | 0.56              |
| 2:J:68:ALA:HB1  | 2:T:47:ILE:O    | 2.06                     | 0.56              |
| 3:K:201:ASN:HA  | 3:K:218:CYS:HA  | 1.87                     | 0.56              |
| 3:BA:201:ASN:HA | 3:BA:218:CYS:HA | 1.87                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:HA:201:ASN:HA | 3:HA:218:CYS:HA | 1.87                     | 0.56              |
| 3:ZA:201:ASN:HA | 3:ZA:218:CYS:HA | 1.88                     | 0.56              |
| 3:LB:201:ASN:HA | 3:LB:218:CYS:HA | 1.88                     | 0.56              |
| 2:QB:74:ASN:CA  | 2:WB:42:ALA:O   | 2.54                     | 0.56              |
| 3:DC:88:PRO:HA  | 3:DC:198:ILE:HA | 1.86                     | 0.56              |
| 3:ZD:201:ASN:HA | 3:ZD:218:CYS:HA | 1.88                     | 0.56              |
| 3:FE:201:ASN:HA | 3:FE:218:CYS:HA | 1.87                     | 0.56              |
| 3:XE:201:ASN:HA | 3:XE:218:CYS:HA | 1.87                     | 0.56              |
| 3:PF:88:PRO:HA  | 3:PF:198:ILE:HA | 1.86                     | 0.56              |
| 2:WB:68:ALA:HB1 | 2:CC:47:ILE:O   | 2.04                     | 0.56              |
| 2:MD:77:LEU:CB  | 2:SD:42:ALA:O   | 2.54                     | 0.56              |
| 3:TD:85:ARG:N   | 3:TD:201:ASN:O  | 2.36                     | 0.56              |
| 2:J:74:ASN:CA   | 2:T:42:ALA:O    | 2.54                     | 0.56              |
| 3:V:201:ASN:HA  | 3:V:218:CYS:HA  | 1.87                     | 0.56              |
| 2:SA:74:ASN:CA  | 2:YA:42:ALA:O   | 2.52                     | 0.56              |
| 3:RE:85:ARG:N   | 3:RE:201:ASN:O  | 2.36                     | 0.56              |
| 3:DF:102:LEU:O  | 3:DF:183:GLU:N  | 2.31                     | 0.56              |
| 3:HG:88:PRO:HA  | 3:HG:198:ILE:HA | 1.86                     | 0.56              |
| 2:G:42:ALA:O    | 2:SG:74:ASN:CA  | 2.52                     | 0.56              |
| 3:M:201:ASN:HA  | 3:M:218:CYS:HA  | 1.87                     | 0.56              |
| 3:ZA:85:ARG:N   | 3:ZA:201:ASN:O  | 2.36                     | 0.56              |
| 3:RE:201:ASN:HA | 3:RE:218:CYS:HA | 1.87                     | 0.56              |
| 3:BG:88:PRO:HA  | 3:BG:198:ILE:HA | 1.86                     | 0.56              |
| 3:BA:88:PRO:HA  | 3:BA:198:ILE:HA | 1.86                     | 0.56              |
| 2:EB:74:ASN:CA  | 2:KB:42:ALA:O   | 2.52                     | 0.56              |
| 3:XB:88:PRO:HA  | 3:XB:198:ILE:HA | 1.86                     | 0.56              |
| 3:JF:201:ASN:HA | 3:JF:218:CYS:HA | 1.87                     | 0.56              |
| 3:C:88:PRO:HA   | 3:C:198:ILE:HA  | 1.86                     | 0.56              |
| 3:TA:85:ARG:N   | 3:TA:201:ASN:O  | 2.36                     | 0.56              |
| 3:LB:85:ARG:N   | 3:LB:201:ASN:O  | 2.36                     | 0.56              |
| 2:SD:68:ALA:HB1 | 2:YD:47:ILE:O   | 2.06                     | 0.56              |
| 2:WE:77:LEU:CB  | 2:CF:42:ALA:O   | 2.54                     | 0.56              |
| 3:DF:201:ASN:HA | 3:DF:218:CYS:HA | 1.87                     | 0.56              |
| 3:VF:201:ASN:HA | 3:VF:218:CYS:HA | 1.87                     | 0.56              |
| 2:GG:77:LEU:CB  | 2:MG:42:ALA:O   | 2.53                     | 0.56              |
| 3:NG:201:ASN:HA | 3:NG:218:CYS:HA | 1.87                     | 0.56              |
| 2:AA:68:ALA:HB1 | 2:GA:47:ILE:O   | 2.05                     | 0.56              |
| 3:BG:201:ASN:HA | 3:BG:218:CYS:HA | 1.87                     | 0.56              |
| 2:MG:68:ALA:HB1 | 2:SG:47:ILE:O   | 2.06                     | 0.56              |
| 3:C:201:ASN:HA  | 3:C:218:CYS:HA  | 1.87                     | 0.56              |
| 3:TA:88:PRO:HA  | 3:TA:198:ILE:HA | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:FB:85:ARG:N    | 3:FB:201:ASN:O   | 2.36                     | 0.56              |
| 2:QB:68:ALA:HB1  | 2:WB:47:ILE:O    | 2.06                     | 0.56              |
| 2:KE:74:ASN:CA   | 2:QE:42:ALA:O    | 2.52                     | 0.56              |
| 3:JF:85:ARG:N    | 3:JF:201:ASN:O   | 2.36                     | 0.56              |
| 3:HG:201:ASN:HA  | 3:HG:218:CYS:HA  | 1.87                     | 0.56              |
| 3:TG:201:ASN:HA  | 3:TG:218:CYS:HA  | 1.87                     | 0.56              |
| 3:JC:85:ARG:N    | 3:JC:201:ASN:O   | 2.36                     | 0.55              |
| 3:XE:102:LEU:O   | 3:XE:183:GLU:N   | 2.31                     | 0.55              |
| 3:PF:201:ASN:HA  | 3:PF:218:CYS:HA  | 1.87                     | 0.55              |
| 3:NG:88:PRO:HA   | 3:NG:198:ILE:HA  | 1.86                     | 0.55              |
| 2:MA:155:HIS:CB  | 2:SA:217:ALA:HB2 | 2.34                     | 0.55              |
| 4:SC:109:GLY:HA3 | 4:SC:122:ILE:HA  | 1.88                     | 0.55              |
| 3:LB:88:PRO:HA   | 3:LB:198:ILE:HA  | 1.86                     | 0.55              |
| 3:DF:85:ARG:N    | 3:DF:201:ASN:O   | 2.36                     | 0.55              |
| 3:NA:85:ARG:N    | 3:NA:201:ASN:O   | 2.36                     | 0.55              |
| 4:YC:109:GLY:HA3 | 4:YC:122:ILE:HA  | 1.88                     | 0.55              |
| 2:KE:77:LEU:CB   | 2:QE:42:ALA:C    | 2.79                     | 0.55              |
| 2:CF:74:ASN:CA   | 2:IF:42:ALA:O    | 2.51                     | 0.55              |
| 4:JA:121:ARG:HA  | 4:KA:86:VAL:HA   | 1.89                     | 0.55              |
| 2:EE:68:ALA:HB1  | 2:KE:47:ILE:O    | 2.06                     | 0.55              |
| 3:PF:85:ARG:N    | 3:PF:201:ASN:O   | 2.36                     | 0.55              |
| 4:KG:109:GLY:HA3 | 4:KG:122:ILE:HA  | 1.88                     | 0.55              |
| 4:NB:121:ARG:HA  | 4:OB:86:VAL:HA   | 1.89                     | 0.55              |
| 4:TB:121:ARG:HA  | 4:UB:86:VAL:HA   | 1.89                     | 0.55              |
| 4:XC:121:ARG:HA  | 4:YC:86:VAL:HA   | 1.89                     | 0.55              |
| 4:EG:109:GLY:HA3 | 4:EG:122:ILE:HA  | 1.88                     | 0.55              |
| 4:Q:109:GLY:HA3  | 4:Q:122:ILE:HA   | 1.88                     | 0.55              |
| 4:IB:109:GLY:HA3 | 4:IB:122:ILE:HA  | 1.88                     | 0.55              |
| 4:OB:109:GLY:HA3 | 4:OB:122:ILE:HA  | 1.88                     | 0.55              |
| 4:MC:109:GLY:HA3 | 4:MC:122:ILE:HA  | 1.88                     | 0.55              |
| 3:ND:85:ARG:N    | 3:ND:201:ASN:O   | 2.36                     | 0.55              |
| 4:MF:109:GLY:HA3 | 4:MF:122:ILE:HA  | 1.88                     | 0.55              |
| 4:SF:109:GLY:HA3 | 4:SF:122:ILE:HA  | 1.88                     | 0.55              |
| 4:H:109:GLY:HA3  | 4:H:122:ILE:HA   | 1.88                     | 0.55              |
| 4:PA:121:ARG:HA  | 4:QA:86:VAL:HA   | 1.89                     | 0.55              |
| 4:ZB:122:ILE:O   | 4:AC:84:GLY:N    | 2.34                     | 0.55              |
| 4:RC:121:ARG:HA  | 4:SC:86:VAL:HA   | 1.89                     | 0.55              |
| 3:RE:102:LEU:O   | 3:RE:183:GLU:N   | 2.31                     | 0.55              |
| 3:XE:85:ARG:N    | 3:XE:201:ASN:O   | 2.36                     | 0.55              |
| 4:WG:109:GLY:HA3 | 4:WG:122:ILE:HA  | 1.88                     | 0.55              |
| 3:ZA:283:VAL:HA  | 4:AB:121:ARG:HA  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:DC:89:TYR:N    | 3:DC:197:ASP:O  | 2.40                     | 0.55              |
| 2:IC:68:ALA:HB1  | 2:OC:47:ILE:O   | 2.07                     | 0.55              |
| 4:DD:121:ARG:HA  | 4:ED:86:VAL:HA  | 1.89                     | 0.55              |
| 4:QG:109:GLY:HA3 | 4:QG:122:ILE:HA | 1.88                     | 0.55              |
| 4:DA:121:ARG:HA  | 4:EA:86:VAL:HA  | 1.89                     | 0.55              |
| 3:TA:270:LEU:O   | 4:UA:62:VAL:N   | 2.27                     | 0.55              |
| 3:TA:283:VAL:HA  | 4:UA:121:ARG:HA | 1.89                     | 0.55              |
| 4:UB:109:GLY:HA3 | 4:UB:122:ILE:HA | 1.88                     | 0.55              |
| 4:ZB:121:ARG:HA  | 4:AC:86:VAL:HA  | 1.89                     | 0.55              |
| 2:IC:74:ASN:CA   | 2:OC:42:ALA:O   | 2.55                     | 0.55              |
| 3:VC:89:TYR:N    | 3:VC:197:ASP:O  | 2.40                     | 0.55              |
| 4:BE:121:ARG:HA  | 4:CE:86:VAL:HA  | 1.89                     | 0.55              |
| 4:YF:109:GLY:HA3 | 4:YF:122:ILE:HA | 1.88                     | 0.55              |
| 4:P:121:ARG:HA   | 4:Q:86:VAL:HA   | 1.89                     | 0.54              |
| 3:V:85:ARG:N     | 3:V:201:ASN:O   | 2.35                     | 0.54              |
| 4:HB:121:ARG:HA  | 4:IB:86:VAL:HA  | 1.89                     | 0.54              |
| 3:LB:89:TYR:N    | 3:LB:197:ASP:O  | 2.40                     | 0.54              |
| 3:RB:283:VAL:HA  | 4:SB:121:ARG:HA | 1.89                     | 0.54              |
| 3:XB:283:VAL:HA  | 4:YB:121:ARG:HA | 1.89                     | 0.54              |
| 3:JC:283:VAL:HA  | 4:KC:121:ARG:HA | 1.89                     | 0.54              |
| 3:PC:283:VAL:HA  | 4:QC:121:ARG:HA | 1.89                     | 0.54              |
| 4:ED:109:GLY:HA3 | 4:ED:122:ILE:HA | 1.88                     | 0.54              |
| 2:GG:183:LEU:O   | 2:GG:187:ASN:N  | 2.41                     | 0.54              |
| 2:MG:183:LEU:O   | 2:MG:187:ASN:N  | 2.41                     | 0.54              |
| 2:SG:183:LEU:O   | 2:SG:187:ASN:N  | 2.41                     | 0.54              |
| 4:Y:109:GLY:HA3  | 4:Y:122:ILE:HA  | 1.88                     | 0.54              |
| 3:BA:283:VAL:HA  | 4:CA:121:ARG:HA | 1.89                     | 0.54              |
| 3:HA:283:VAL:HA  | 4:IA:121:ARG:HA | 1.89                     | 0.54              |
| 3:FB:283:VAL:HA  | 4:GB:121:ARG:HA | 1.89                     | 0.54              |
| 3:LB:283:VAL:HA  | 4:MB:121:ARG:HA | 1.89                     | 0.54              |
| 3:ND:89:TYR:N    | 3:ND:197:ASP:O  | 2.40                     | 0.54              |
| 2:YD:183:LEU:O   | 2:YD:187:ASN:N  | 2.41                     | 0.54              |
| 4:CE:109:GLY:HA3 | 4:CE:122:ILE:HA | 1.88                     | 0.54              |
| 4:HE:121:ARG:HA  | 4:IE:86:VAL:HA  | 1.89                     | 0.54              |
| 4:UE:109:GLY:HA3 | 4:UE:122:ILE:HA | 1.88                     | 0.54              |
| 4:AF:109:GLY:HA3 | 4:AF:122:ILE:HA | 1.88                     | 0.54              |
| 2:G:183:LEU:O    | 2:G:187:ASN:N   | 2.41                     | 0.54              |
| 4:R:109:GLY:HA3  | 4:R:122:ILE:HA  | 1.88                     | 0.54              |
| 4:CB:109:GLY:HA3 | 4:CB:122:ILE:HA | 1.88                     | 0.54              |
| 3:DC:283:VAL:HA  | 4:EC:121:ARG:HA | 1.89                     | 0.54              |
| 4:FC:122:ILE:O   | 4:GC:84:GLY:N   | 2.34                     | 0.54              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:LC:121:ARG:HA  | 4:MC:86:VAL:HA  | 1.89                     | 0.54              |
| 2:OC:139:ARG:C   | 2:UC:205:LEU:CB | 2.81                     | 0.54              |
| 3:HD:270:LEU:O   | 4:ID:62:VAL:N   | 2.27                     | 0.54              |
| 2:SD:183:LEU:O   | 2:SD:187:ASN:N  | 2.41                     | 0.54              |
| 4:VD:121:ARG:HA  | 4:WD:86:VAL:HA  | 1.89                     | 0.54              |
| 4:WD:109:GLY:HA3 | 4:WD:122:ILE:HA | 1.88                     | 0.54              |
| 2:EE:183:LEU:O   | 2:EE:187:ASN:N  | 2.41                     | 0.54              |
| 2:AG:183:LEU:O   | 2:AG:187:ASN:N  | 2.41                     | 0.54              |
| 4:E:121:ARG:HA   | 4:H:86:VAL:HA   | 1.89                     | 0.54              |
| 3:K:85:ARG:N     | 3:K:201:ASN:O   | 2.36                     | 0.54              |
| 3:NA:283:VAL:HA  | 4:OA:121:ARG:HA | 1.89                     | 0.54              |
| 4:VA:121:ARG:HA  | 4:WA:86:VAL:HA  | 1.89                     | 0.54              |
| 4:GC:109:GLY:HA3 | 4:GC:122:ILE:HA | 1.88                     | 0.54              |
| 3:LE:102:LEU:O   | 3:LE:183:GLU:N  | 2.31                     | 0.54              |
| 3:VF:85:ARG:N    | 3:VF:201:ASN:O  | 2.36                     | 0.54              |
| 3:BA:85:ARG:N    | 3:BA:201:ASN:O  | 2.36                     | 0.54              |
| 4:EA:109:GLY:HA3 | 4:EA:122:ILE:HA | 1.88                     | 0.54              |
| 3:TA:89:TYR:N    | 3:TA:197:ASP:O  | 2.40                     | 0.54              |
| 3:VC:270:LEU:O   | 4:WC:62:VAL:N   | 2.27                     | 0.54              |
| 4:XC:122:ILE:O   | 4:YC:84:GLY:N   | 2.34                     | 0.54              |
| 2:MD:183:LEU:O   | 2:MD:187:ASN:N  | 2.41                     | 0.54              |
| 3:FE:89:TYR:N    | 3:FE:197:ASP:O  | 2.40                     | 0.54              |
| 4:GF:109:GLY:HA3 | 4:GF:122:ILE:HA | 1.88                     | 0.54              |
| 3:NG:85:ARG:N    | 3:NG:201:ASN:O  | 2.36                     | 0.54              |
| 4:VG:121:ARG:HA  | 4:WG:86:VAL:HA  | 1.89                     | 0.54              |
| 2:B:183:LEU:O    | 2:B:187:ASN:N   | 2.41                     | 0.54              |
| 3:K:283:VAL:HA   | 4:L:121:ARG:HA  | 1.89                     | 0.54              |
| 2:MA:77:LEU:CB   | 2:SA:42:ALA:O   | 2.55                     | 0.54              |
| 4:RC:122:ILE:O   | 4:SC:84:GLY:N   | 2.34                     | 0.54              |
| 2:OF:183:LEU:O   | 2:OF:187:ASN:N  | 2.41                     | 0.54              |
| 2:UF:183:LEU:O   | 2:UF:187:ASN:N  | 2.41                     | 0.54              |
| 3:HG:85:ARG:N    | 3:HG:201:ASN:O  | 2.36                     | 0.54              |
| 3:HA:85:ARG:N    | 3:HA:201:ASN:O  | 2.36                     | 0.54              |
| 3:VC:283:VAL:HA  | 4:WC:121:ARG:HA | 1.89                     | 0.54              |
| 4:JD:121:ARG:HA  | 4:KD:86:VAL:HA  | 1.89                     | 0.54              |
| 3:TD:270:LEU:O   | 4:UD:62:VAL:N   | 2.27                     | 0.54              |
| 4:IE:109:GLY:HA3 | 4:IE:122:ILE:HA | 1.88                     | 0.54              |
| 2:KE:139:ARG:C   | 2:QE:205:LEU:CB | 2.80                     | 0.54              |
| 2:KE:183:LEU:O   | 2:KE:187:ASN:N  | 2.41                     | 0.54              |
| 4:NE:121:ARG:HA  | 4:OE:86:VAL:HA  | 1.89                     | 0.54              |
| 2:QE:183:LEU:O   | 2:QE:187:ASN:N  | 2.41                     | 0.54              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:XE:270:LEU:O   | 4:YE:62:VAL:N   | 2.27                     | 0.54              |
| 2:CF:183:LEU:O   | 2:CF:187:ASN:N  | 2.41                     | 0.54              |
| 2:IF:183:LEU:O   | 2:IF:187:ASN:N  | 2.41                     | 0.54              |
| 3:C:283:VAL:HA   | 4:D:121:ARG:HA  | 1.89                     | 0.54              |
| 2:J:183:LEU:O    | 2:J:187:ASN:N   | 2.41                     | 0.54              |
| 3:V:283:VAL:HA   | 4:W:121:ARG:HA  | 1.89                     | 0.54              |
| 4:KA:109:GLY:HA3 | 4:KA:122:ILE:HA | 1.88                     | 0.54              |
| 3:BD:283:VAL:HA  | 4:CD:121:ARG:HA | 1.89                     | 0.54              |
| 2:GD:183:LEU:O   | 2:GD:187:ASN:N  | 2.41                     | 0.54              |
| 3:HD:283:VAL:HA  | 4:ID:121:ARG:HA | 1.89                     | 0.54              |
| 4:QD:109:GLY:HA3 | 4:QD:122:ILE:HA | 1.88                     | 0.54              |
| 4:OE:109:GLY:HA3 | 4:OE:122:ILE:HA | 1.88                     | 0.54              |
| 2:WE:183:LEU:O   | 2:WE:187:ASN:N  | 2.41                     | 0.54              |
| 3:XE:89:TYR:N    | 3:XE:197:ASP:O  | 2.40                     | 0.54              |
| 3:JF:51:LEU:HA   | 3:JF:232:VAL:HA | 1.90                     | 0.54              |
| 4:LF:121:ARG:HA  | 4:MF:86:VAL:HA  | 1.89                     | 0.54              |
| 3:PF:283:VAL:HA  | 4:QF:121:ARG:HA | 1.89                     | 0.54              |
| 4:RF:121:ARG:HA  | 4:SF:86:VAL:HA  | 1.89                     | 0.54              |
| 2:T:183:LEU:O    | 2:T:187:ASN:N   | 2.41                     | 0.54              |
| 3:HA:51:LEU:HA   | 3:HA:232:VAL:HA | 1.90                     | 0.54              |
| 3:HA:270:LEU:O   | 4:IA:62:VAL:N   | 2.27                     | 0.54              |
| 3:TA:51:LEU:HA   | 3:TA:232:VAL:HA | 1.90                     | 0.54              |
| 2:YA:68:ALA:HB1  | 2:EB:47:ILE:O   | 2.08                     | 0.54              |
| 3:ZA:51:LEU:HA   | 3:ZA:232:VAL:HA | 1.90                     | 0.54              |
| 3:LB:51:LEU:HA   | 3:LB:232:VAL:HA | 1.90                     | 0.54              |
| 4:AC:109:GLY:HA3 | 4:AC:122:ILE:HA | 1.88                     | 0.54              |
| 4:LC:122:ILE:O   | 4:MC:84:GLY:N   | 2.34                     | 0.54              |
| 3:RE:51:LEU:HA   | 3:RE:232:VAL:HA | 1.90                     | 0.54              |
| 3:XE:283:VAL:HA  | 4:YE:121:ARG:HA | 1.89                     | 0.54              |
| 3:VF:51:LEU:HA   | 3:VF:232:VAL:HA | 1.90                     | 0.54              |
| 3:BG:51:LEU:HA   | 3:BG:232:VAL:HA | 1.90                     | 0.54              |
| 2:MG:74:ASN:CA   | 2:SG:42:ALA:O   | 2.54                     | 0.54              |
| 4:PG:121:ARG:HA  | 4:QG:86:VAL:HA  | 1.89                     | 0.54              |
| 3:TG:51:LEU:HA   | 3:TG:232:VAL:HA | 1.90                     | 0.54              |
| 3:TG:85:ARG:N    | 3:TG:201:ASN:O  | 2.36                     | 0.54              |
| 3:K:51:LEU:HA    | 3:K:232:VAL:HA  | 1.90                     | 0.54              |
| 4:O:121:ARG:HA   | 4:R:86:VAL:HA   | 1.89                     | 0.54              |
| 4:X:121:ARG:HA   | 4:Y:86:VAL:HA   | 1.89                     | 0.54              |
| 2:AA:183:LEU:O   | 2:AA:187:ASN:N  | 2.41                     | 0.54              |
| 3:BA:51:LEU:HA   | 3:BA:232:VAL:HA | 1.90                     | 0.54              |
| 2:GA:183:LEU:O   | 2:GA:187:ASN:N  | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:DC:51:LEU:HA   | 3:DC:232:VAL:HA  | 1.90                     | 0.54              |
| 3:DC:85:ARG:N    | 3:DC:201:ASN:O   | 2.36                     | 0.54              |
| 3:JC:270:LEU:O   | 4:KC:62:VAL:N    | 2.27                     | 0.54              |
| 2:AD:183:LEU:O   | 2:AD:187:ASN:N   | 2.41                     | 0.54              |
| 4:PD:121:ARG:HA  | 4:QD:86:VAL:HA   | 1.89                     | 0.54              |
| 3:RE:283:VAL:HA  | 4:SE:121:ARG:HA  | 1.89                     | 0.54              |
| 3:DF:51:LEU:HA   | 3:DF:232:VAL:HA  | 1.90                     | 0.54              |
| 3:PF:89:TYR:N    | 3:PF:197:ASP:O   | 2.40                     | 0.54              |
| 3:NG:51:LEU:HA   | 3:NG:232:VAL:HA  | 1.90                     | 0.54              |
| 3:M:283:VAL:HA   | 4:N:121:ARG:HA   | 1.89                     | 0.53              |
| 3:C:51:LEU:HA    | 3:C:232:VAL:HA   | 1.90                     | 0.53              |
| 3:C:85:ARG:N     | 3:C:201:ASN:O    | 2.35                     | 0.53              |
| 4:FC:121:ARG:HA  | 4:GC:86:VAL:HA   | 1.89                     | 0.53              |
| 2:OC:77:LEU:CB   | 2:UC:42:ALA:C    | 2.82                     | 0.53              |
| 2:UC:183:LEU:O   | 2:UC:187:ASN:N   | 2.41                     | 0.53              |
| 3:ZD:51:LEU:HA   | 3:ZD:232:VAL:HA  | 1.90                     | 0.53              |
| 3:FE:102:LEU:O   | 3:FE:183:GLU:N   | 2.31                     | 0.53              |
| 3:DF:283:VAL:HA  | 4:EF:121:ARG:HA  | 1.89                     | 0.53              |
| 3:VF:283:VAL:HA  | 4:WF:121:ARG:HA  | 1.89                     | 0.53              |
| 4:XF:121:ARG:HA  | 4:YF:86:VAL:HA   | 1.89                     | 0.53              |
| 3:BA:89:TYR:N    | 3:BA:197:ASP:O   | 2.40                     | 0.53              |
| 2:MA:183:LEU:O   | 2:MA:187:ASN:N   | 2.41                     | 0.53              |
| 4:QA:109:GLY:HA3 | 4:QA:122:ILE:HA  | 1.88                     | 0.53              |
| 2:YA:77:LEU:CB   | 2:EB:42:ALA:C    | 2.81                     | 0.53              |
| 4:BB:121:ARG:HA  | 4:CB:86:VAL:HA   | 1.89                     | 0.53              |
| 2:IC:77:LEU:CB   | 2:OC:42:ALA:C    | 2.81                     | 0.53              |
| 2:OC:183:LEU:O   | 2:OC:187:ASN:N   | 2.40                     | 0.53              |
| 2:AD:77:LEU:CB   | 2:GD:42:ALA:C    | 2.82                     | 0.53              |
| 4:KD:109:GLY:HA3 | 4:KD:122:ILE:HA  | 1.88                     | 0.53              |
| 3:ND:283:VAL:HA  | 4:OD:121:ARG:HA  | 1.89                     | 0.53              |
| 2:EE:218:VAL:O   | 2:EE:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:JF:283:VAL:HA  | 4:KF:121:ARG:HA  | 1.89                     | 0.53              |
| 3:HG:89:TYR:N    | 3:HG:197:ASP:O   | 2.40                     | 0.53              |
| 2:T:218:VAL:O    | 2:T:226:ALA:HB2  | 2.09                     | 0.53              |
| 3:V:89:TYR:N     | 3:V:197:ASP:O    | 2.40                     | 0.53              |
| 2:SA:183:LEU:O   | 2:SA:187:ASN:N   | 2.41                     | 0.53              |
| 4:WA:109:GLY:HA3 | 4:WA:122:ILE:HA  | 1.88                     | 0.53              |
| 3:RB:51:LEU:HA   | 3:RB:232:VAL:HA  | 1.90                     | 0.53              |
| 3:RB:89:TYR:N    | 3:RB:197:ASP:O   | 2.40                     | 0.53              |
| 3:VC:51:LEU:HA   | 3:VC:232:VAL:HA  | 1.90                     | 0.53              |
| 3:HD:85:ARG:N    | 3:HD:201:ASN:O   | 2.36                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:FE:283:VAL:HA | 4:GE:121:ARG:HA  | 1.89                     | 0.53              |
| 4:FF:121:ARG:HA | 4:GF:86:VAL:HA   | 1.89                     | 0.53              |
| 3:NG:283:VAL:HA | 4:OG:121:ARG:HA  | 1.89                     | 0.53              |
| 3:TG:283:VAL:HA | 4:UG:121:ARG:HA  | 1.89                     | 0.53              |
| 2:J:218:VAL:O   | 2:J:226:ALA:HB2  | 2.09                     | 0.53              |
| 2:WB:183:LEU:O  | 2:WB:187:ASN:N   | 2.40                     | 0.53              |
| 2:IC:183:LEU:O  | 2:IC:187:ASN:N   | 2.41                     | 0.53              |
| 3:JC:89:TYR:N   | 3:JC:197:ASP:O   | 2.40                     | 0.53              |
| 2:UC:218:VAL:O  | 2:UC:226:ALA:HB2 | 2.09                     | 0.53              |
| 2:SD:74:ASN:CA  | 2:YD:42:ALA:O    | 2.54                     | 0.53              |
| 2:EE:74:ASN:CA  | 2:KE:42:ALA:O    | 2.54                     | 0.53              |
| 2:KE:218:VAL:O  | 2:KE:226:ALA:HB2 | 2.09                     | 0.53              |
| 2:IF:218:VAL:O  | 2:IF:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:BG:85:ARG:N   | 3:BG:201:ASN:O   | 2.36                     | 0.53              |
| 3:HG:283:VAL:HA | 4:IG:121:ARG:HA  | 1.89                     | 0.53              |
| 3:C:89:TYR:N    | 3:C:197:ASP:O    | 2.40                     | 0.53              |
| 3:V:270:LEU:O   | 4:W:62:VAL:N     | 2.27                     | 0.53              |
| 2:AA:218:VAL:O  | 2:AA:226:ALA:HB2 | 2.09                     | 0.53              |
| 2:YA:183:LEU:O  | 2:YA:187:ASN:N   | 2.41                     | 0.53              |
| 2:EB:183:LEU:O  | 2:EB:187:ASN:N   | 2.41                     | 0.53              |
| 2:EB:218:VAL:O  | 2:EB:226:ALA:HB2 | 2.09                     | 0.53              |
| 2:KB:183:LEU:O  | 2:KB:187:ASN:N   | 2.41                     | 0.53              |
| 2:KB:218:VAL:O  | 2:KB:226:ALA:HB2 | 2.09                     | 0.53              |
| 2:QB:183:LEU:O  | 2:QB:187:ASN:N   | 2.41                     | 0.53              |
| 2:CC:183:LEU:O  | 2:CC:187:ASN:N   | 2.41                     | 0.53              |
| 2:OC:218:VAL:O  | 2:OC:226:ALA:HB2 | 2.09                     | 0.53              |
| 2:AD:218:VAL:O  | 2:AD:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:HD:51:LEU:HA  | 3:HD:232:VAL:HA  | 1.90                     | 0.53              |
| 3:ND:51:LEU:HA  | 3:ND:232:VAL:HA  | 1.90                     | 0.53              |
| 3:TD:283:VAL:HA | 4:UD:121:ARG:HA  | 1.89                     | 0.53              |
| 2:YD:218:VAL:O  | 2:YD:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:ZD:283:VAL:HA | 4:AE:121:ARG:HA  | 1.89                     | 0.53              |
| 3:LE:51:LEU:HA  | 3:LE:232:VAL:HA  | 1.90                     | 0.53              |
| 3:LE:283:VAL:HA | 4:ME:121:ARG:HA  | 1.89                     | 0.53              |
| 3:BG:283:VAL:HA | 4:CG:121:ARG:HA  | 1.89                     | 0.53              |
| 2:MG:218:VAL:O  | 2:MG:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:HA:89:TYR:N   | 3:HA:197:ASP:O   | 2.40                     | 0.53              |
| 3:FE:270:LEU:O  | 4:GE:62:VAL:N    | 2.27                     | 0.53              |
| 2:OF:218:VAL:O  | 2:OF:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:BG:89:TYR:N   | 3:BG:197:ASP:O   | 2.40                     | 0.53              |
| 2:GG:218:VAL:O  | 2:GG:226:ALA:HB2 | 2.09                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:YA:218:VAL:O  | 2:YA:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:ZA:89:TYR:N   | 3:ZA:197:ASP:O   | 2.40                     | 0.53              |
| 4:ZE:121:ARG:HA | 4:AF:86:VAL:HA   | 1.89                     | 0.53              |
| 2:CF:218:VAL:O  | 2:CF:226:ALA:HB2 | 2.09                     | 0.53              |
| 2:IF:77:LEU:CB  | 2:OF:42:ALA:C    | 2.82                     | 0.53              |
| 2:SG:218:VAL:O  | 2:SG:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:M:85:ARG:N    | 3:M:201:ASN:O    | 2.36                     | 0.53              |
| 3:XB:270:LEU:O  | 4:YB:62:VAL:N    | 2.27                     | 0.53              |
| 3:PC:51:LEU:HA  | 3:PC:232:VAL:HA  | 1.90                     | 0.53              |
| 3:BD:89:TYR:N   | 3:BD:197:ASP:O   | 2.40                     | 0.53              |
| 4:JG:121:ARG:HA | 4:KG:86:VAL:HA   | 1.89                     | 0.53              |
| 3:C:270:LEU:O   | 4:D:62:VAL:N     | 2.27                     | 0.53              |
| 2:KB:77:LEU:CB  | 2:QB:42:ALA:O    | 2.56                     | 0.53              |
| 3:ZD:102:LEU:O  | 3:ZD:183:GLU:N   | 2.31                     | 0.53              |
| 3:FE:51:LEU:HA  | 3:FE:232:VAL:HA  | 1.90                     | 0.53              |
| 4:TE:121:ARG:HA | 4:UE:86:VAL:HA   | 1.89                     | 0.53              |
| 4:DG:121:ARG:HA | 4:EG:86:VAL:HA   | 1.89                     | 0.53              |
| 2:B:218:VAL:O   | 2:B:226:ALA:HB2  | 2.09                     | 0.53              |
| 2:QB:218:VAL:O  | 2:QB:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:JC:51:LEU:HA  | 3:JC:232:VAL:HA  | 1.90                     | 0.53              |
| 2:QE:218:VAL:O  | 2:QE:226:ALA:HB2 | 2.09                     | 0.53              |
| 3:XE:51:LEU:HA  | 3:XE:232:VAL:HA  | 1.90                     | 0.53              |
| 3:TG:89:TYR:N   | 3:TG:197:ASP:O   | 2.40                     | 0.53              |
| 2:GA:218:VAL:O  | 2:GA:226:ALA:HB2 | 2.09                     | 0.52              |
| 2:SA:218:VAL:O  | 2:SA:226:ALA:HB2 | 2.09                     | 0.52              |
| 3:XB:51:LEU:HA  | 3:XB:232:VAL:HA  | 1.90                     | 0.52              |
| 2:IC:218:VAL:O  | 2:IC:226:ALA:HB2 | 2.09                     | 0.52              |
| 2:GD:218:VAL:O  | 2:GD:226:ALA:HB2 | 2.09                     | 0.52              |
| 2:SD:218:VAL:O  | 2:SD:226:ALA:HB2 | 2.09                     | 0.52              |
| 4:TB:122:ILE:O  | 4:UB:84:GLY:N    | 2.34                     | 0.52              |
| 3:PF:51:LEU:HA  | 3:PF:232:VAL:HA  | 1.90                     | 0.52              |
| 2:AG:218:VAL:O  | 2:AG:226:ALA:HB2 | 2.09                     | 0.52              |
| 3:M:51:LEU:HA   | 3:M:232:VAL:HA   | 1.90                     | 0.52              |
| 3:V:51:LEU:HA   | 3:V:232:VAL:HA   | 1.90                     | 0.52              |
| 3:NA:51:LEU:HA  | 3:NA:232:VAL:HA  | 1.90                     | 0.52              |
| 2:WB:77:LEU:CB  | 2:CC:42:ALA:C    | 2.82                     | 0.52              |
| 3:TD:51:LEU:HA  | 3:TD:232:VAL:HA  | 1.90                     | 0.52              |
| 3:TD:89:TYR:N   | 3:TD:197:ASP:O   | 2.40                     | 0.52              |
| 2:IF:68:ALA:HB1 | 2:OF:47:ILE:O    | 2.09                     | 0.52              |
| 2:UF:218:VAL:O  | 2:UF:226:ALA:HB2 | 2.09                     | 0.52              |
| 3:FB:51:LEU:HA  | 3:FB:232:VAL:HA  | 1.90                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:HG:51:LEU:HA  | 3:HG:232:VAL:HA  | 1.90                     | 0.52              |
| 2:T:219:ARG:CA  | 2:T:226:ALA:CB   | 2.88                     | 0.52              |
| 2:YA:74:ASN:CA  | 2:EB:42:ALA:O    | 2.56                     | 0.52              |
| 2:WE:218:VAL:O  | 2:WE:226:ALA:HB2 | 2.09                     | 0.52              |
| 3:JF:270:LEU:O  | 4:KF:62:VAL:N    | 2.27                     | 0.52              |
| 3:NG:89:TYR:N   | 3:NG:197:ASP:O   | 2.40                     | 0.52              |
| 2:G:42:ALA:C    | 2:SG:77:LEU:CB   | 2.82                     | 0.52              |
| 2:J:219:ARG:CA  | 2:J:226:ALA:CB   | 2.88                     | 0.52              |
| 2:AA:219:ARG:CA | 2:AA:226:ALA:CB  | 2.88                     | 0.52              |
| 2:GA:219:ARG:CA | 2:GA:226:ALA:CB  | 2.88                     | 0.52              |
| 3:LE:89:TYR:N   | 3:LE:197:ASP:O   | 2.40                     | 0.52              |
| 3:BG:270:LEU:O  | 4:CG:62:VAL:N    | 2.27                     | 0.52              |
| 2:G:218:VAL:O   | 2:G:226:ALA:HB2  | 2.09                     | 0.52              |
| 2:G:219:ARG:CA  | 2:G:226:ALA:CB   | 2.88                     | 0.52              |
| 2:B:219:ARG:CA  | 2:B:226:ALA:CB   | 2.88                     | 0.52              |
| 2:J:77:LEU:CB   | 2:T:42:ALA:C     | 2.82                     | 0.52              |
| 2:GA:77:LEU:CB  | 2:MA:42:ALA:C    | 2.82                     | 0.52              |
| 2:MA:219:ARG:CA | 2:MA:226:ALA:CB  | 2.88                     | 0.52              |
| 3:LB:270:LEU:O  | 4:MB:62:VAL:N    | 2.27                     | 0.52              |
| 3:TD:102:LEU:O  | 3:TD:183:GLU:N   | 2.31                     | 0.52              |
| 3:K:270:LEU:O   | 4:L:62:VAL:N     | 2.27                     | 0.52              |
| 2:SA:219:ARG:CA | 2:SA:226:ALA:CB  | 2.88                     | 0.52              |
| 2:YA:219:ARG:CA | 2:YA:226:ALA:CB  | 2.88                     | 0.52              |
| 3:DF:89:TYR:N   | 3:DF:197:ASP:O   | 2.40                     | 0.52              |
| 2:SG:219:ARG:CA | 2:SG:226:ALA:CB  | 2.88                     | 0.52              |
| 2:WB:218:VAL:O  | 2:WB:226:ALA:HB2 | 2.09                     | 0.52              |
| 3:BD:51:LEU:HA  | 3:BD:232:VAL:HA  | 1.90                     | 0.52              |
| 2:MD:218:VAL:O  | 2:MD:226:ALA:HB2 | 2.09                     | 0.52              |
| 3:RE:270:LEU:O  | 4:SE:62:VAL:N    | 2.27                     | 0.52              |
| 3:VF:89:TYR:N   | 3:VF:197:ASP:O   | 2.40                     | 0.52              |
| 2:MG:219:ARG:CA | 2:MG:226:ALA:CB  | 2.88                     | 0.52              |
| 2:MA:218:VAL:O  | 2:MA:226:ALA:HB2 | 2.09                     | 0.52              |
| 2:EB:219:ARG:CA | 2:EB:226:ALA:CB  | 2.88                     | 0.52              |
| 2:KB:219:ARG:CA | 2:KB:226:ALA:CB  | 2.88                     | 0.52              |
| 2:CC:218:VAL:O  | 2:CC:226:ALA:HB2 | 2.09                     | 0.52              |
| 2:AD:139:ARG:C  | 2:GD:205:LEU:CB  | 2.83                     | 0.52              |
| 2:IF:219:ARG:N  | 2:IF:226:ALA:CB  | 2.74                     | 0.51              |
| 3:NA:89:TYR:N   | 3:NA:197:ASP:O   | 2.40                     | 0.51              |
| 2:QB:219:ARG:CA | 2:QB:226:ALA:CB  | 2.88                     | 0.51              |
| 2:KE:219:ARG:HA | 2:KE:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:CF:219:ARG:HA | 2:CF:226:ALA:HB3 | 1.93                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:UF:219:ARG:N  | 2:UF:226:ALA:CB  | 2.74                     | 0.51              |
| 2:GG:219:ARG:CA | 2:GG:226:ALA:CB  | 2.88                     | 0.51              |
| 2:SD:219:ARG:HA | 2:SD:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:QE:219:ARG:N  | 2:QE:226:ALA:CB  | 2.74                     | 0.51              |
| 2:WE:219:ARG:N  | 2:WE:226:ALA:CB  | 2.74                     | 0.51              |
| 2:CF:219:ARG:N  | 2:CF:226:ALA:CB  | 2.74                     | 0.51              |
| 2:OF:219:ARG:N  | 2:OF:226:ALA:CB  | 2.74                     | 0.51              |
| 2:AG:219:ARG:N  | 2:AG:226:ALA:CB  | 2.74                     | 0.51              |
| 2:GA:139:ARG:C  | 2:MA:205:LEU:CB  | 2.83                     | 0.51              |
| 2:WB:219:ARG:CA | 2:WB:226:ALA:CB  | 2.88                     | 0.51              |
| 2:OF:77:LEU:CB  | 2:UF:42:ALA:C    | 2.84                     | 0.51              |
| 2:UF:219:ARG:HA | 2:UF:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:GG:219:ARG:N  | 2:GG:226:ALA:CB  | 2.74                     | 0.51              |
| 3:ZA:270:LEU:O  | 4:AB:62:VAL:N    | 2.27                     | 0.51              |
| 2:OC:219:ARG:N  | 2:OC:226:ALA:CB  | 2.74                     | 0.51              |
| 2:UC:219:ARG:N  | 2:UC:226:ALA:CB  | 2.74                     | 0.51              |
| 3:BD:85:ARG:N   | 3:BD:201:ASN:O   | 2.36                     | 0.51              |
| 2:KE:219:ARG:N  | 2:KE:226:ALA:CB  | 2.74                     | 0.51              |
| 2:KE:219:ARG:CA | 2:KE:226:ALA:CB  | 2.88                     | 0.51              |
| 2:QE:219:ARG:CA | 2:QE:226:ALA:CB  | 2.88                     | 0.51              |
| 2:CF:219:ARG:CA | 2:CF:226:ALA:CB  | 2.88                     | 0.51              |
| 2:AG:77:LEU:CB  | 2:GG:42:ALA:C    | 2.83                     | 0.51              |
| 2:AG:219:ARG:CA | 2:AG:226:ALA:CB  | 2.88                     | 0.51              |
| 3:K:89:TYR:N    | 3:K:197:ASP:O    | 2.40                     | 0.51              |
| 2:EE:219:ARG:N  | 2:EE:226:ALA:CB  | 2.74                     | 0.51              |
| 2:EE:219:ARG:HA | 2:EE:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:EE:219:ARG:CA | 2:EE:226:ALA:CB  | 2.88                     | 0.51              |
| 2:WE:219:ARG:HA | 2:WE:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:WE:219:ARG:CA | 2:WE:226:ALA:CB  | 2.88                     | 0.51              |
| 2:T:219:ARG:N   | 2:T:226:ALA:CB   | 2.74                     | 0.51              |
| 2:AA:219:ARG:N  | 2:AA:226:ALA:CB  | 2.74                     | 0.51              |
| 2:EB:77:LEU:CB  | 2:KB:42:ALA:C    | 2.83                     | 0.51              |
| 3:XB:89:TYR:N   | 3:XB:197:ASP:O   | 2.40                     | 0.51              |
| 2:CC:219:ARG:CA | 2:CC:226:ALA:CB  | 2.88                     | 0.51              |
| 2:IC:219:ARG:N  | 2:IC:226:ALA:CB  | 2.74                     | 0.51              |
| 2:AD:219:ARG:N  | 2:AD:226:ALA:CB  | 2.74                     | 0.51              |
| 2:AD:219:ARG:HA | 2:AD:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:MD:219:ARG:HA | 2:MD:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:IF:219:ARG:CA | 2:IF:226:ALA:CB  | 2.88                     | 0.51              |
| 2:OF:219:ARG:HA | 2:OF:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:UF:219:ARG:CA | 2:UF:226:ALA:CB  | 2.88                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:MG:219:ARG:N  | 2:MG:226:ALA:CB  | 2.74                     | 0.51              |
| 3:NG:270:LEU:O  | 4:OG:62:VAL:N    | 2.27                     | 0.51              |
| 2:GA:219:ARG:N  | 2:GA:226:ALA:CB  | 2.74                     | 0.51              |
| 3:FB:89:TYR:N   | 3:FB:197:ASP:O   | 2.40                     | 0.51              |
| 2:CC:219:ARG:N  | 2:CC:226:ALA:CB  | 2.74                     | 0.51              |
| 2:OC:219:ARG:CA | 2:OC:226:ALA:CB  | 2.88                     | 0.51              |
| 2:UC:219:ARG:CA | 2:UC:226:ALA:CB  | 2.88                     | 0.51              |
| 2:GD:219:ARG:N  | 2:GD:226:ALA:CB  | 2.74                     | 0.51              |
| 2:YD:219:ARG:CA | 2:YD:226:ALA:CB  | 2.88                     | 0.51              |
| 3:RE:89:TYR:N   | 3:RE:197:ASP:O   | 2.40                     | 0.51              |
| 2:MG:219:ARG:HA | 2:MG:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:T:77:LEU:CB   | 2:AA:42:ALA:C    | 2.83                     | 0.51              |
| 2:MA:219:ARG:N  | 2:MA:226:ALA:CB  | 2.74                     | 0.51              |
| 2:WB:139:ARG:C  | 2:CC:205:LEU:CB  | 2.84                     | 0.51              |
| 2:AD:219:ARG:CA | 2:AD:226:ALA:CB  | 2.88                     | 0.51              |
| 2:GD:219:ARG:CA | 2:GD:226:ALA:CB  | 2.88                     | 0.51              |
| 2:MD:219:ARG:CA | 2:MD:226:ALA:CB  | 2.88                     | 0.51              |
| 2:SD:219:ARG:CA | 2:SD:226:ALA:CB  | 2.88                     | 0.51              |
| 2:YD:219:ARG:N  | 2:YD:226:ALA:CB  | 2.74                     | 0.51              |
| 2:OF:219:ARG:CA | 2:OF:226:ALA:CB  | 2.88                     | 0.51              |
| 3:BG:102:LEU:O  | 3:BG:183:GLU:N   | 2.31                     | 0.51              |
| 2:GG:219:ARG:HA | 2:GG:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:J:219:ARG:N   | 2:J:226:ALA:CB   | 2.74                     | 0.51              |
| 2:IC:219:ARG:HA | 2:IC:226:ALA:HB3 | 1.93                     | 0.51              |
| 2:IC:219:ARG:CA | 2:IC:226:ALA:CB  | 2.88                     | 0.51              |
| 2:UC:219:ARG:HA | 2:UC:226:ALA:HB3 | 1.92                     | 0.51              |
| 2:G:205:LEU:CB  | 2:SG:139:ARG:C   | 2.84                     | 0.50              |
| 2:J:119:ALA:O   | 2:J:123:ARG:N    | 2.44                     | 0.50              |
| 2:AA:119:ALA:O  | 2:AA:123:ARG:N   | 2.44                     | 0.50              |
| 2:SA:119:ALA:O  | 2:SA:123:ARG:N   | 2.44                     | 0.50              |
| 2:SA:219:ARG:N  | 2:SA:226:ALA:CB  | 2.74                     | 0.50              |
| 2:WB:119:ALA:O  | 2:WB:123:ARG:N   | 2.44                     | 0.50              |
| 2:OC:119:ALA:O  | 2:OC:123:ARG:N   | 2.44                     | 0.50              |
| 3:PC:89:TYR:N   | 3:PC:197:ASP:O   | 2.40                     | 0.50              |
| 2:AD:119:ALA:O  | 2:AD:123:ARG:N   | 2.44                     | 0.50              |
| 2:GD:119:ALA:O  | 2:GD:123:ARG:N   | 2.44                     | 0.50              |
| 2:SG:119:ALA:O  | 2:SG:123:ARG:N   | 2.44                     | 0.50              |
| 2:SG:219:ARG:N  | 2:SG:226:ALA:CB  | 2.74                     | 0.50              |
| 2:B:219:ARG:N   | 2:B:226:ALA:CB   | 2.74                     | 0.50              |
| 2:AA:77:LEU:CB  | 2:GA:42:ALA:C    | 2.84                     | 0.50              |
| 3:NA:270:LEU:O  | 4:OA:62:VAL:N    | 2.27                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:WB:219:ARG:N  | 2:WB:226:ALA:CB  | 2.74                     | 0.50              |
| 2:MD:219:ARG:N  | 2:MD:226:ALA:CB  | 2.74                     | 0.50              |
| 3:VF:270:LEU:O  | 4:WF:62:VAL:N    | 2.27                     | 0.50              |
| 2:G:219:ARG:HA  | 2:G:226:ALA:HB3  | 1.93                     | 0.50              |
| 2:B:119:ALA:O   | 2:B:123:ARG:N    | 2.44                     | 0.50              |
| 3:K:200:VAL:N   | 3:K:219:LEU:O    | 2.44                     | 0.50              |
| 3:BA:200:VAL:N  | 3:BA:219:LEU:O   | 2.44                     | 0.50              |
| 2:GA:119:ALA:O  | 2:GA:123:ARG:N   | 2.44                     | 0.50              |
| 2:KB:119:ALA:O  | 2:KB:123:ARG:N   | 2.44                     | 0.50              |
| 2:SD:219:ARG:N  | 2:SD:226:ALA:CB  | 2.74                     | 0.50              |
| 3:HG:102:LEU:O  | 3:HG:183:GLU:N   | 2.31                     | 0.50              |
| 3:M:270:LEU:O   | 4:N:62:VAL:N     | 2.27                     | 0.50              |
| 2:B:77:LEU:CB   | 2:J:42:ALA:C     | 2.84                     | 0.50              |
| 3:V:200:VAL:N   | 3:V:219:LEU:O    | 2.44                     | 0.50              |
| 3:HA:200:VAL:N  | 3:HA:219:LEU:O   | 2.44                     | 0.50              |
| 2:EB:119:ALA:O  | 2:EB:123:ARG:N   | 2.44                     | 0.50              |
| 2:IC:119:ALA:O  | 2:IC:123:ARG:N   | 2.44                     | 0.50              |
| 2:OC:139:ARG:O  | 2:UC:205:LEU:CB  | 2.60                     | 0.50              |
| 2:YD:119:ALA:O  | 2:YD:123:ARG:N   | 2.44                     | 0.50              |
| 2:QE:219:ARG:HA | 2:QE:226:ALA:HB3 | 1.93                     | 0.50              |
| 2:IF:219:ARG:HA | 2:IF:226:ALA:HB3 | 1.93                     | 0.50              |
| 2:G:219:ARG:N   | 2:G:226:ALA:CB   | 2.74                     | 0.50              |
| 3:C:200:VAL:N   | 3:C:219:LEU:O    | 2.44                     | 0.50              |
| 2:T:219:ARG:HA  | 2:T:226:ALA:HB3  | 1.92                     | 0.50              |
| 2:QB:219:ARG:HA | 2:QB:226:ALA:HB3 | 1.93                     | 0.50              |
| 2:YD:219:ARG:HA | 2:YD:226:ALA:HB3 | 1.93                     | 0.50              |
| 3:M:200:VAL:N   | 3:M:219:LEU:O    | 2.44                     | 0.50              |
| 2:B:219:ARG:HA  | 2:B:226:ALA:HB3  | 1.93                     | 0.50              |
| 3:NA:200:VAL:N  | 3:NA:219:LEU:O   | 2.44                     | 0.50              |
| 2:SA:77:LEU:CB  | 2:YA:42:ALA:C    | 2.84                     | 0.50              |
| 3:TA:200:VAL:N  | 3:TA:219:LEU:O   | 2.44                     | 0.50              |
| 2:YA:219:ARG:N  | 2:YA:226:ALA:CB  | 2.74                     | 0.50              |
| 2:QB:219:ARG:N  | 2:QB:226:ALA:CB  | 2.74                     | 0.50              |
| 2:GD:77:LEU:CB  | 2:MD:42:ALA:C    | 2.85                     | 0.50              |
| 2:GD:219:ARG:HA | 2:GD:226:ALA:HB3 | 1.93                     | 0.50              |
| 2:SD:77:LEU:CB  | 2:YD:42:ALA:C    | 2.85                     | 0.50              |
| 2:QE:77:LEU:CB  | 2:WE:42:ALA:C    | 2.85                     | 0.50              |
| 3:DF:270:LEU:O  | 4:EF:62:VAL:N    | 2.27                     | 0.50              |
| 3:NG:102:LEU:O  | 3:NG:183:GLU:N   | 2.31                     | 0.50              |
| 4:O:119:GLY:HA2 | 4:R:88:ALA:HA    | 1.94                     | 0.50              |
| 3:BA:270:LEU:O  | 4:CA:62:VAL:N    | 2.27                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:TB:119:GLY:HA2 | 4:UB:88:ALA:HA   | 1.94                     | 0.50              |
| 2:CC:119:ALA:O   | 2:CC:123:ARG:N   | 2.44                     | 0.50              |
| 4:LC:119:GLY:HA2 | 4:MC:88:ALA:HA   | 1.94                     | 0.50              |
| 2:OC:219:ARG:HA  | 2:OC:226:ALA:HB3 | 1.92                     | 0.50              |
| 2:IF:74:ASN:CA   | 2:OF:42:ALA:O    | 2.57                     | 0.50              |
| 1:NF:552:ARG:HA  | 2:OF:67:ALA:HB2  | 1.94                     | 0.50              |
| 4:JA:119:GLY:HA2 | 4:KA:88:ALA:HA   | 1.94                     | 0.50              |
| 2:YA:219:ARG:HA  | 2:YA:226:ALA:HB3 | 1.93                     | 0.50              |
| 3:ZA:200:VAL:N   | 3:ZA:219:LEU:O   | 2.44                     | 0.50              |
| 4:BB:119:GLY:HA2 | 4:CB:88:ALA:HA   | 1.94                     | 0.50              |
| 2:IC:139:ARG:C   | 2:OC:205:LEU:CB  | 2.85                     | 0.50              |
| 3:HD:89:TYR:N    | 3:HD:197:ASP:O   | 2.40                     | 0.50              |
| 1:JE:552:ARG:HA  | 2:KE:67:ALA:HB2  | 1.94                     | 0.50              |
| 1:VE:552:ARG:HA  | 2:WE:67:ALA:HB2  | 1.94                     | 0.50              |
| 1:HF:552:ARG:HA  | 2:IF:67:ALA:HB2  | 1.94                     | 0.50              |
| 1:ZF:552:ARG:HA  | 2:AG:67:ALA:HB2  | 1.94                     | 0.50              |
| 2:AG:219:ARG:HA  | 2:AG:226:ALA:HB3 | 1.93                     | 0.50              |
| 3:TG:200:VAL:N   | 3:TG:219:LEU:O   | 2.44                     | 0.50              |
| 4:VG:119:GLY:HA2 | 4:WG:88:ALA:HA   | 1.94                     | 0.50              |
| 2:GA:219:ARG:HA  | 2:GA:226:ALA:HB3 | 1.92                     | 0.50              |
| 2:MA:119:ALA:O   | 2:MA:123:ARG:N   | 2.44                     | 0.50              |
| 2:YA:119:ALA:O   | 2:YA:123:ARG:N   | 2.44                     | 0.50              |
| 2:YA:139:ARG:C   | 2:EB:205:LEU:CB  | 2.85                     | 0.50              |
| 1:XD:552:ARG:HA  | 2:YD:67:ALA:HB2  | 1.94                     | 0.50              |
| 1:DE:552:ARG:HA  | 2:EE:67:ALA:HB2  | 1.94                     | 0.50              |
| 2:CF:77:LEU:CB   | 2:IF:42:ALA:C    | 2.85                     | 0.50              |
| 2:OF:139:ARG:C   | 2:UF:205:LEU:CB  | 2.85                     | 0.50              |
| 2:AG:139:ARG:C   | 2:GG:205:LEU:CB  | 2.85                     | 0.50              |
| 2:MA:219:ARG:HA  | 2:MA:226:ALA:HB3 | 1.93                     | 0.49              |
| 2:EB:219:ARG:N   | 2:EB:226:ALA:CB  | 2.74                     | 0.49              |
| 2:WB:219:ARG:HA  | 2:WB:226:ALA:HB3 | 1.93                     | 0.49              |
| 4:DD:119:GLY:HA2 | 4:ED:88:ALA:HA   | 1.94                     | 0.49              |
| 3:ZD:89:TYR:N    | 3:ZD:197:ASP:O   | 2.40                     | 0.49              |
| 1:PE:552:ARG:HA  | 2:QE:67:ALA:HB2  | 1.94                     | 0.49              |
| 1:BF:552:ARG:HA  | 2:CF:67:ALA:HB2  | 1.94                     | 0.49              |
| 3:JF:200:VAL:N   | 3:JF:219:LEU:O   | 2.44                     | 0.49              |
| 3:PF:200:VAL:N   | 3:PF:219:LEU:O   | 2.44                     | 0.49              |
| 1:TF:552:ARG:HA  | 2:UF:67:ALA:HB2  | 1.94                     | 0.49              |
| 3:NG:200:VAL:N   | 3:NG:219:LEU:O   | 2.44                     | 0.49              |
| 2:G:119:ALA:O    | 2:G:123:ARG:N    | 2.44                     | 0.49              |
| 3:M:89:TYR:N     | 3:M:197:ASP:O    | 2.40                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:PA:119:GLY:HA2 | 4:QA:88:ALA:HA   | 1.94                     | 0.49              |
| 2:EB:219:ARG:HA  | 2:EB:226:ALA:HB3 | 1.93                     | 0.49              |
| 3:FB:200:VAL:N   | 3:FB:219:LEU:O   | 2.44                     | 0.49              |
| 2:KB:219:ARG:N   | 2:KB:226:ALA:CB  | 2.74                     | 0.49              |
| 2:CC:219:ARG:HA  | 2:CC:226:ALA:HB3 | 1.93                     | 0.49              |
| 3:ND:270:LEU:O   | 4:OD:62:VAL:N    | 2.27                     | 0.49              |
| 3:DF:200:VAL:N   | 3:DF:219:LEU:O   | 2.44                     | 0.49              |
| 3:JF:89:TYR:N    | 3:JF:197:ASP:O   | 2.40                     | 0.49              |
| 1:LG:552:ARG:HA  | 2:MG:67:ALA:HB2  | 1.94                     | 0.49              |
| 2:QB:119:ALA:O   | 2:QB:123:ARG:N   | 2.44                     | 0.49              |
| 4:ZB:119:GLY:HA2 | 4:AC:88:ALA:HA   | 1.94                     | 0.49              |
| 2:UC:119:ALA:O   | 2:UC:123:ARG:N   | 2.44                     | 0.49              |
| 3:BD:270:LEU:O   | 4:CD:62:VAL:N    | 2.27                     | 0.49              |
| 1:LD:552:ARG:HA  | 2:MD:67:ALA:HB2  | 1.94                     | 0.49              |
| 3:VF:200:VAL:N   | 3:VF:219:LEU:O   | 2.44                     | 0.49              |
| 3:BG:200:VAL:N   | 3:BG:219:LEU:O   | 2.44                     | 0.49              |
| 1:FG:552:ARG:HA  | 2:GG:67:ALA:HB2  | 1.94                     | 0.49              |
| 4:P:119:GLY:HA2  | 4:Q:88:ALA:HA    | 1.94                     | 0.49              |
| 2:T:119:ALA:O    | 2:T:123:ARG:N    | 2.44                     | 0.49              |
| 4:X:119:GLY:HA2  | 4:Y:88:ALA:HA    | 1.94                     | 0.49              |
| 2:AA:219:ARG:HA  | 2:AA:226:ALA:HB3 | 1.93                     | 0.49              |
| 4:HB:119:GLY:HA2 | 4:IB:88:ALA:HA   | 1.94                     | 0.49              |
| 1:FD:552:ARG:HA  | 2:GD:67:ALA:HB2  | 1.94                     | 0.49              |
| 1:RD:552:ARG:HA  | 2:SD:67:ALA:HB2  | 1.94                     | 0.49              |
| 3:RE:200:VAL:N   | 3:RE:219:LEU:O   | 2.44                     | 0.49              |
| 3:XE:200:VAL:N   | 3:XE:219:LEU:O   | 2.44                     | 0.49              |
| 2:GG:119:ALA:O   | 2:GG:123:ARG:N   | 2.44                     | 0.49              |
| 3:HG:200:VAL:N   | 3:HG:219:LEU:O   | 2.44                     | 0.49              |
| 1:F:552:ARG:HA   | 2:G:67:ALA:HB2   | 1.94                     | 0.49              |
| 3:LB:200:VAL:N   | 3:LB:219:LEU:O   | 2.44                     | 0.49              |
| 2:WB:63:ALA:HA   | 2:WB:67:ALA:HB3  | 1.94                     | 0.49              |
| 4:RC:119:GLY:HA2 | 4:SC:88:ALA:HA   | 1.94                     | 0.49              |
| 2:UC:63:ALA:HA   | 2:UC:67:ALA:HB3  | 1.94                     | 0.49              |
| 4:VD:119:GLY:HA2 | 4:WD:88:ALA:HA   | 1.94                     | 0.49              |
| 4:DG:119:GLY:HA2 | 4:EG:88:ALA:HA   | 1.94                     | 0.49              |
| 4:JG:119:GLY:HA2 | 4:KG:88:ALA:HA   | 1.94                     | 0.49              |
| 1:RG:552:ARG:HA  | 2:SG:67:ALA:HB2  | 1.94                     | 0.49              |
| 2:YA:63:ALA:HA   | 2:YA:67:ALA:HB3  | 1.94                     | 0.49              |
| 3:XB:301:VAL:O   | 3:XB:321:ILE:N   | 2.45                     | 0.49              |
| 3:DC:301:VAL:O   | 3:DC:321:ILE:N   | 2.45                     | 0.49              |
| 2:IC:63:ALA:HA   | 2:IC:67:ALA:HB3  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:PC:301:VAL:O   | 3:PC:321:ILE:N   | 2.45                     | 0.49              |
| 3:VC:301:VAL:O   | 3:VC:321:ILE:N   | 2.45                     | 0.49              |
| 1:ZC:552:ARG:HA  | 2:AD:67:ALA:HB2  | 1.94                     | 0.49              |
| 3:ZD:270:LEU:O   | 4:AE:62:VAL:N    | 2.27                     | 0.49              |
| 3:LE:200:VAL:N   | 3:LE:219:LEU:O   | 2.44                     | 0.49              |
| 4:RF:119:GLY:HA2 | 4:SF:88:ALA:HA   | 1.94                     | 0.49              |
| 2:UF:77:LEU:CB   | 2:AG:42:ALA:C    | 2.86                     | 0.49              |
| 2:SG:219:ARG:HA  | 2:SG:226:ALA:HB3 | 1.93                     | 0.49              |
| 1:A:552:ARG:HA   | 2:B:67:ALA:HB2   | 1.94                     | 0.49              |
| 2:T:139:ARG:C    | 2:AA:205:LEU:CB  | 2.85                     | 0.49              |
| 4:W:111:VAL:HA   | 4:W:120:VAL:HA   | 1.95                     | 0.49              |
| 2:SA:219:ARG:HA  | 2:SA:226:ALA:HB3 | 1.93                     | 0.49              |
| 2:KB:63:ALA:HA   | 2:KB:67:ALA:HB3  | 1.95                     | 0.49              |
| 3:RB:200:VAL:N   | 3:RB:219:LEU:O   | 2.44                     | 0.49              |
| 3:JC:301:VAL:O   | 3:JC:321:ILE:N   | 2.45                     | 0.49              |
| 3:BD:301:VAL:O   | 3:BD:321:ILE:N   | 2.45                     | 0.49              |
| 3:HD:301:VAL:O   | 3:HD:321:ILE:N   | 2.45                     | 0.49              |
| 4:ZE:119:GLY:HA2 | 4:AF:88:ALA:HA   | 1.94                     | 0.49              |
| 2:IF:139:ARG:C   | 2:OF:205:LEU:CB  | 2.86                     | 0.49              |
| 2:J:219:ARG:HA   | 2:J:226:ALA:HB3  | 1.93                     | 0.49              |
| 4:DA:119:GLY:HA2 | 4:EA:88:ALA:HA   | 1.94                     | 0.49              |
| 4:VA:119:GLY:HA2 | 4:WA:88:ALA:HA   | 1.94                     | 0.49              |
| 2:EB:63:ALA:HA   | 2:EB:67:ALA:HB3  | 1.94                     | 0.49              |
| 3:RB:301:VAL:O   | 3:RB:321:ILE:N   | 2.45                     | 0.49              |
| 2:CC:63:ALA:HA   | 2:CC:67:ALA:HB3  | 1.94                     | 0.49              |
| 1:NC:552:ARG:HA  | 2:OC:67:ALA:HB2  | 1.94                     | 0.49              |
| 1:TC:552:ARG:HA  | 2:UC:67:ALA:HB2  | 1.94                     | 0.49              |
| 2:MD:119:ALA:O   | 2:MD:123:ARG:N   | 2.44                     | 0.49              |
| 3:ND:301:VAL:O   | 3:ND:321:ILE:N   | 2.45                     | 0.49              |
| 3:TD:301:VAL:O   | 3:TD:321:ILE:N   | 2.45                     | 0.49              |
| 3:FE:200:VAL:N   | 3:FE:219:LEU:O   | 2.44                     | 0.49              |
| 4:D:111:VAL:HA   | 4:D:120:VAL:HA   | 1.95                     | 0.49              |
| 1:I:552:ARG:HA   | 2:J:67:ALA:HB2   | 1.94                     | 0.49              |
| 4:L:111:VAL:HA   | 4:L:120:VAL:HA   | 1.95                     | 0.49              |
| 4:CA:111:VAL:HA  | 4:CA:120:VAL:HA  | 1.95                     | 0.49              |
| 4:IA:111:VAL:HA  | 4:IA:120:VAL:HA  | 1.95                     | 0.49              |
| 4:OA:111:VAL:HA  | 4:OA:120:VAL:HA  | 1.95                     | 0.49              |
| 4:UA:111:VAL:HA  | 4:UA:120:VAL:HA  | 1.95                     | 0.49              |
| 3:FB:80:THR:O    | 3:FB:205:HIS:N   | 2.35                     | 0.49              |
| 3:LB:301:VAL:O   | 3:LB:321:ILE:N   | 2.45                     | 0.49              |
| 4:NB:119:GLY:HA2 | 4:OB:88:ALA:HA   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:MC:110:GLU:O   | 4:MC:121:ARG:N   | 2.42                     | 0.49              |
| 3:PC:270:LEU:O   | 4:QC:62:VAL:N    | 2.27                     | 0.49              |
| 2:GD:63:ALA:HA   | 2:GD:67:ALA:HB3  | 1.94                     | 0.49              |
| 4:PD:119:GLY:HA2 | 4:QD:88:ALA:HA   | 1.94                     | 0.49              |
| 2:EE:77:LEU:CB   | 2:KE:42:ALA:C    | 2.85                     | 0.49              |
| 4:HE:119:GLY:HA2 | 4:IE:88:ALA:HA   | 1.94                     | 0.49              |
| 4:NE:119:GLY:HA2 | 4:OE:88:ALA:HA   | 1.94                     | 0.49              |
| 2:AG:63:ALA:HA   | 2:AG:67:ALA:HB3  | 1.95                     | 0.49              |
| 4:N:111:VAL:HA   | 4:N:120:VAL:HA   | 1.95                     | 0.49              |
| 2:QB:63:ALA:HA   | 2:QB:67:ALA:HB3  | 1.95                     | 0.49              |
| 3:RB:270:LEU:O   | 4:SB:62:VAL:N    | 2.27                     | 0.49              |
| 3:XB:200:VAL:N   | 3:XB:219:LEU:O   | 2.44                     | 0.49              |
| 4:FC:119:GLY:HA2 | 4:GC:88:ALA:HA   | 1.94                     | 0.49              |
| 3:VC:85:ARG:N    | 3:VC:201:ASN:O   | 2.36                     | 0.49              |
| 4:XC:119:GLY:HA2 | 4:YC:88:ALA:HA   | 1.94                     | 0.49              |
| 3:ZD:200:VAL:N   | 3:ZD:219:LEU:O   | 2.44                     | 0.49              |
| 3:ZD:301:VAL:O   | 3:ZD:321:ILE:N   | 2.45                     | 0.49              |
| 2:UF:63:ALA:HA   | 2:UF:67:ALA:HB3  | 1.94                     | 0.49              |
| 3:HG:270:LEU:O   | 4:IG:62:VAL:N    | 2.27                     | 0.49              |
| 4:UG:111:VAL:HA  | 4:UG:120:VAL:HA  | 1.95                     | 0.49              |
| 4:E:119:GLY:HA2  | 4:H:88:ALA:HA    | 1.94                     | 0.48              |
| 1:Z:552:ARG:HA   | 2:AA:67:ALA:HB2  | 1.94                     | 0.48              |
| 2:EB:139:ARG:C   | 2:KB:205:LEU:CB  | 2.86                     | 0.48              |
| 3:FB:301:VAL:O   | 3:FB:321:ILE:N   | 2.45                     | 0.48              |
| 1:BC:552:ARG:HA  | 2:CC:67:ALA:HB2  | 1.94                     | 0.48              |
| 3:DC:200:VAL:N   | 3:DC:219:LEU:O   | 2.44                     | 0.48              |
| 4:GC:110:GLU:O   | 4:GC:121:ARG:N   | 2.42                     | 0.48              |
| 1:HC:552:ARG:HA  | 2:IC:67:ALA:HB2  | 1.94                     | 0.48              |
| 2:OC:63:ALA:HA   | 2:OC:67:ALA:HB3  | 1.95                     | 0.48              |
| 2:AD:63:ALA:HA   | 2:AD:67:ALA:HB3  | 1.95                     | 0.48              |
| 4:JD:119:GLY:HA2 | 4:KD:88:ALA:HA   | 1.94                     | 0.48              |
| 2:EE:119:ALA:O   | 2:EE:123:ARG:N   | 2.44                     | 0.48              |
| 2:WE:119:ALA:O   | 2:WE:123:ARG:N   | 2.44                     | 0.48              |
| 4:LF:119:GLY:HA2 | 4:MF:88:ALA:HA   | 1.94                     | 0.48              |
| 2:J:139:ARG:C    | 2:T:205:LEU:CB   | 2.85                     | 0.48              |
| 1:S:552:ARG:HA   | 2:T:67:ALA:HB2   | 1.94                     | 0.48              |
| 4:GB:111:VAL:HA  | 4:GB:120:VAL:HA  | 1.95                     | 0.48              |
| 2:KB:219:ARG:HA  | 2:KB:226:ALA:HB3 | 1.93                     | 0.48              |
| 4:OB:110:GLU:O   | 4:OB:121:ARG:N   | 2.42                     | 0.48              |
| 4:UB:110:GLU:O   | 4:UB:121:ARG:N   | 2.42                     | 0.48              |
| 4:AC:110:GLU:O   | 4:AC:121:ARG:N   | 2.42                     | 0.48              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:GG:77:LEU:CB   | 2:MG:42:ALA:C   | 2.86                     | 0.48              |
| 4:IG:111:VAL:HA  | 4:IG:120:VAL:HA | 1.95                     | 0.48              |
| 4:OG:111:VAL:HA  | 4:OG:120:VAL:HA | 1.95                     | 0.48              |
| 2:B:63:ALA:HA    | 2:B:67:ALA:HB3  | 1.95                     | 0.48              |
| 1:FA:552:ARG:HA  | 2:GA:67:ALA:HB2 | 1.94                     | 0.48              |
| 2:MA:63:ALA:HA   | 2:MA:67:ALA:HB3 | 1.95                     | 0.48              |
| 3:ZA:301:VAL:O   | 3:ZA:321:ILE:N  | 2.45                     | 0.48              |
| 4:AB:111:VAL:HA  | 4:AB:120:VAL:HA | 1.95                     | 0.48              |
| 2:KB:77:LEU:CB   | 2:QB:42:ALA:C   | 2.86                     | 0.48              |
| 1:PB:552:ARG:HA  | 2:QB:67:ALA:HB2 | 1.94                     | 0.48              |
| 1:VB:552:ARG:HA  | 2:WB:67:ALA:HB2 | 1.94                     | 0.48              |
| 2:CC:77:LEU:CB   | 2:IC:42:ALA:C   | 2.86                     | 0.48              |
| 3:JC:200:VAL:N   | 3:JC:219:LEU:O  | 2.44                     | 0.48              |
| 2:MD:63:ALA:HA   | 2:MD:67:ALA:HB3 | 1.94                     | 0.48              |
| 3:ND:200:VAL:N   | 3:ND:219:LEU:O  | 2.44                     | 0.48              |
| 2:SD:63:ALA:HA   | 2:SD:67:ALA:HB3 | 1.95                     | 0.48              |
| 3:TD:200:VAL:N   | 3:TD:219:LEU:O  | 2.44                     | 0.48              |
| 3:FE:301:VAL:O   | 3:FE:321:ILE:N  | 2.45                     | 0.48              |
| 4:CG:111:VAL:HA  | 4:CG:120:VAL:HA | 1.95                     | 0.48              |
| 2:GG:63:ALA:HA   | 2:GG:67:ALA:HB3 | 1.94                     | 0.48              |
| 2:G:63:ALA:HA    | 2:G:67:ALA:HB3  | 1.95                     | 0.48              |
| 3:BA:80:THR:O    | 3:BA:205:HIS:N  | 2.35                     | 0.48              |
| 3:TA:301:VAL:O   | 3:TA:321:ILE:N  | 2.45                     | 0.48              |
| 4:CB:110:GLU:O   | 4:CB:121:ARG:N  | 2.42                     | 0.48              |
| 1:DB:552:ARG:HA  | 2:EB:67:ALA:HB2 | 1.94                     | 0.48              |
| 4:IB:110:GLU:O   | 4:IB:121:ARG:N  | 2.42                     | 0.48              |
| 2:KB:139:ARG:C   | 2:QB:205:LEU:CB | 2.86                     | 0.48              |
| 4:MB:111:VAL:HA  | 4:MB:120:VAL:HA | 1.95                     | 0.48              |
| 4:SB:111:VAL:HA  | 4:SB:120:VAL:HA | 1.95                     | 0.48              |
| 3:PC:200:VAL:N   | 3:PC:219:LEU:O  | 2.44                     | 0.48              |
| 3:HD:200:VAL:N   | 3:HD:219:LEU:O  | 2.44                     | 0.48              |
| 2:YD:77:LEU:CB   | 2:EE:42:ALA:C   | 2.86                     | 0.48              |
| 3:LE:301:VAL:O   | 3:LE:321:ILE:N  | 2.45                     | 0.48              |
| 2:WE:63:ALA:HA   | 2:WE:67:ALA:HB3 | 1.95                     | 0.48              |
| 4:WF:111:VAL:HA  | 4:WF:120:VAL:HA | 1.95                     | 0.48              |
| 1:LA:552:ARG:HA  | 2:MA:67:ALA:HB2 | 1.94                     | 0.48              |
| 1:JB:552:ARG:HA  | 2:KB:67:ALA:HB2 | 1.94                     | 0.48              |
| 3:VC:200:VAL:N   | 3:VC:219:LEU:O  | 2.44                     | 0.48              |
| 3:BD:200:VAL:N   | 3:BD:219:LEU:O  | 2.44                     | 0.48              |
| 3:LE:270:LEU:O   | 4:ME:62:VAL:N   | 2.27                     | 0.48              |
| 4:FF:119:GLY:HA2 | 4:GF:88:ALA:HA  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:OF:63:ALA:HA   | 2:OF:67:ALA:HB3 | 1.94                     | 0.48              |
| 4:PG:119:GLY:HA2 | 4:QG:88:ALA:HA  | 1.94                     | 0.48              |
| 3:NA:301:VAL:O   | 3:NA:321:ILE:N  | 2.45                     | 0.48              |
| 2:SA:63:ALA:HA   | 2:SA:67:ALA:HB3 | 1.95                     | 0.48              |
| 4:WA:110:GLU:O   | 4:WA:121:ARG:N  | 2.42                     | 0.48              |
| 1:XA:552:ARG:HA  | 2:YA:67:ALA:HB2 | 1.94                     | 0.48              |
| 2:QE:63:ALA:HA   | 2:QE:67:ALA:HB3 | 1.95                     | 0.48              |
| 3:RE:301:VAL:O   | 3:RE:321:ILE:N  | 2.45                     | 0.48              |
| 2:MG:77:LEU:CB   | 2:SG:42:ALA:C   | 2.86                     | 0.48              |
| 4:KA:100:LEU:HA  | 4:KA:105:LEU:HA | 1.96                     | 0.48              |
| 1:RA:552:ARG:HA  | 2:SA:67:ALA:HB2 | 1.94                     | 0.48              |
| 4:WA:100:LEU:HA  | 4:WA:105:LEU:HA | 1.96                     | 0.48              |
| 3:DC:270:LEU:O   | 4:EC:62:VAL:N   | 2.27                     | 0.48              |
| 2:YD:63:ALA:HA   | 2:YD:67:ALA:HB3 | 1.95                     | 0.48              |
| 2:KE:139:ARG:O   | 2:QE:205:LEU:CB | 2.61                     | 0.48              |
| 3:PF:270:LEU:O   | 4:QF:62:VAL:N   | 2.27                     | 0.48              |
| 2:J:63:ALA:HA    | 2:J:67:ALA:HB3  | 1.95                     | 0.48              |
| 4:QA:110:GLU:O   | 4:QA:121:ARG:N  | 2.42                     | 0.48              |
| 4:IB:100:LEU:HA  | 4:IB:105:LEU:HA | 1.96                     | 0.48              |
| 4:UB:100:LEU:HA  | 4:UB:105:LEU:HA | 1.96                     | 0.48              |
| 4:YB:111:VAL:HA  | 4:YB:120:VAL:HA | 1.95                     | 0.48              |
| 4:AE:111:VAL:HA  | 4:AE:120:VAL:HA | 1.95                     | 0.48              |
| 4:TE:119:GLY:HA2 | 4:UE:88:ALA:HA  | 1.94                     | 0.48              |
| 4:KF:111:VAL:HA  | 4:KF:120:VAL:HA | 1.95                     | 0.48              |
| 2:G:77:LEU:CB    | 2:B:42:ALA:C    | 2.87                     | 0.48              |
| 2:B:139:ARG:C    | 2:J:205:LEU:CB  | 2.87                     | 0.48              |
| 2:AA:63:ALA:HA   | 2:AA:67:ALA:HB3 | 1.95                     | 0.48              |
| 4:EA:100:LEU:HA  | 4:EA:105:LEU:HA | 1.96                     | 0.48              |
| 2:GA:63:ALA:HA   | 2:GA:67:ALA:HB3 | 1.95                     | 0.48              |
| 3:HA:301:VAL:O   | 3:HA:321:ILE:N  | 2.45                     | 0.48              |
| 4:KA:110:GLU:O   | 4:KA:121:ARG:N  | 2.42                     | 0.48              |
| 4:CB:100:LEU:HA  | 4:CB:105:LEU:HA | 1.96                     | 0.48              |
| 4:OB:100:LEU:HA  | 4:OB:105:LEU:HA | 1.96                     | 0.48              |
| 2:EE:63:ALA:HA   | 2:EE:67:ALA:HB3 | 1.95                     | 0.48              |
| 3:RE:80:THR:O    | 3:RE:205:HIS:N  | 2.35                     | 0.48              |
| 3:XE:301:VAL:O   | 3:XE:321:ILE:N  | 2.45                     | 0.48              |
| 2:CF:63:ALA:HA   | 2:CF:67:ALA:HB3 | 1.95                     | 0.48              |
| 2:SG:63:ALA:HA   | 2:SG:67:ALA:HB3 | 1.94                     | 0.48              |
| 4:H:100:LEU:HA   | 4:H:105:LEU:HA  | 1.96                     | 0.48              |
| 4:R:100:LEU:HA   | 4:R:105:LEU:HA  | 1.96                     | 0.48              |
| 4:BE:119:GLY:HA2 | 4:CE:88:ALA:HA  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:QF:111:VAL:HA  | 4:QF:120:VAL:HA | 1.95                     | 0.48              |
| 4:XF:119:GLY:HA2 | 4:YF:88:ALA:HA  | 1.94                     | 0.48              |
| 4:Q:100:LEU:HA   | 4:Q:105:LEU:HA  | 1.96                     | 0.47              |
| 3:BA:301:VAL:O   | 3:BA:321:ILE:N  | 2.45                     | 0.47              |
| 4:EA:110:GLU:O   | 4:EA:121:ARG:N  | 2.42                     | 0.47              |
| 4:AC:100:LEU:HA  | 4:AC:105:LEU:HA | 1.96                     | 0.47              |
| 2:AD:139:ARG:O   | 2:GD:205:LEU:CB | 2.62                     | 0.47              |
| 4:UD:111:VAL:HA  | 4:UD:120:VAL:HA | 1.95                     | 0.47              |
| 2:KE:63:ALA:HA   | 2:KE:67:ALA:HB3 | 1.94                     | 0.47              |
| 4:YE:111:VAL:HA  | 4:YE:120:VAL:HA | 1.95                     | 0.47              |
| 3:DF:301:VAL:O   | 3:DF:321:ILE:N  | 2.45                     | 0.47              |
| 4:Y:100:LEU:HA   | 4:Y:105:LEU:HA  | 1.96                     | 0.47              |
| 2:QB:77:LEU:CB   | 2:WB:42:ALA:C   | 2.87                     | 0.47              |
| 4:EC:111:VAL:HA  | 4:EC:120:VAL:HA | 1.95                     | 0.47              |
| 4:KC:111:VAL:HA  | 4:KC:120:VAL:HA | 1.95                     | 0.47              |
| 4:MC:100:LEU:HA  | 4:MC:105:LEU:HA | 1.96                     | 0.47              |
| 4:SC:100:LEU:HA  | 4:SC:105:LEU:HA | 1.96                     | 0.47              |
| 4:WC:111:VAL:HA  | 4:WC:120:VAL:HA | 1.95                     | 0.47              |
| 4:GE:111:VAL:HA  | 4:GE:120:VAL:HA | 1.95                     | 0.47              |
| 2:CF:119:ALA:O   | 2:CF:123:ARG:N  | 2.44                     | 0.47              |
| 2:OF:119:ALA:O   | 2:OF:123:ARG:N  | 2.44                     | 0.47              |
| 2:MG:63:ALA:HA   | 2:MG:67:ALA:HB3 | 1.94                     | 0.47              |
| 4:QA:100:LEU:HA  | 4:QA:105:LEU:HA | 1.96                     | 0.47              |
| 2:EB:200:ALA:HB3 | 2:EB:232:GLU:CB | 2.32                     | 0.47              |
| 2:YD:139:ARG:C   | 2:EE:205:LEU:CB | 2.88                     | 0.47              |
| 3:XE:80:THR:O    | 3:XE:205:HIS:N  | 2.35                     | 0.47              |
| 4:EF:111:VAL:HA  | 4:EF:120:VAL:HA | 1.95                     | 0.47              |
| 3:V:301:VAL:O    | 3:V:321:ILE:N   | 2.45                     | 0.47              |
| 4:Y:110:GLU:O    | 4:Y:121:ARG:N   | 2.42                     | 0.47              |
| 4:GC:100:LEU:HA  | 4:GC:105:LEU:HA | 1.96                     | 0.47              |
| 4:CD:111:VAL:HA  | 4:CD:120:VAL:HA | 1.95                     | 0.47              |
| 4:ME:111:VAL:HA  | 4:ME:120:VAL:HA | 1.95                     | 0.47              |
| 2:QE:119:ALA:O   | 2:QE:123:ARG:N  | 2.44                     | 0.47              |
| 2:IF:119:ALA:O   | 2:IF:123:ARG:N  | 2.44                     | 0.47              |
| 3:JF:301:VAL:O   | 3:JF:321:ILE:N  | 2.45                     | 0.47              |
| 2:AG:119:ALA:O   | 2:AG:123:ARG:N  | 2.44                     | 0.47              |
| 2:SG:200:ALA:HB3 | 2:SG:232:GLU:CB | 2.32                     | 0.47              |
| 4:QC:111:VAL:HA  | 4:QC:120:VAL:HA | 1.95                     | 0.47              |
| 2:UC:77:LEU:CB   | 2:AD:42:ALA:C   | 2.88                     | 0.47              |
| 4:QG:100:LEU:HA  | 4:QG:105:LEU:HA | 1.96                     | 0.47              |
| 3:TG:270:LEU:O   | 4:UG:62:VAL:N   | 2.27                     | 0.47              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:K:301:VAL:O    | 3:K:321:ILE:N   | 2.45                     | 0.47              |
| 2:T:63:ALA:HA    | 2:T:67:ALA:HB3  | 1.95                     | 0.47              |
| 2:YA:139:ARG:CB  | 2:EB:205:LEU:CB | 2.92                     | 0.47              |
| 2:GD:139:ARG:C   | 2:MD:205:LEU:CB | 2.88                     | 0.47              |
| 4:KD:100:LEU:HA  | 4:KD:105:LEU:HA | 1.96                     | 0.47              |
| 2:KE:119:ALA:O   | 2:KE:123:ARG:N  | 2.44                     | 0.47              |
| 2:IF:63:ALA:HA   | 2:IF:67:ALA:HB3 | 1.95                     | 0.47              |
| 4:WG:100:LEU:HA  | 4:WG:105:LEU:HA | 1.96                     | 0.47              |
| 3:M:301:VAL:O    | 3:M:321:ILE:N   | 2.45                     | 0.47              |
| 3:C:301:VAL:O    | 3:C:321:ILE:N   | 2.45                     | 0.47              |
| 2:AA:139:ARG:C   | 2:GA:205:LEU:CB | 2.87                     | 0.47              |
| 2:AA:200:ALA:HB3 | 2:AA:232:GLU:CB | 2.32                     | 0.47              |
| 2:KB:139:ARG:O   | 2:QB:205:LEU:CB | 2.63                     | 0.47              |
| 4:YC:100:LEU:HA  | 4:YC:105:LEU:HA | 1.96                     | 0.47              |
| 4:ED:100:LEU:HA  | 4:ED:105:LEU:HA | 1.96                     | 0.47              |
| 4:ID:111:VAL:HA  | 4:ID:120:VAL:HA | 1.95                     | 0.47              |
| 4:OD:111:VAL:HA  | 4:OD:120:VAL:HA | 1.95                     | 0.47              |
| 4:QD:100:LEU:HA  | 4:QD:105:LEU:HA | 1.96                     | 0.47              |
| 4:SE:111:VAL:HA  | 4:SE:120:VAL:HA | 1.95                     | 0.47              |
| 2:WE:77:LEU:CB   | 2:CF:42:ALA:C   | 2.88                     | 0.47              |
| 2:IF:139:ARG:CB  | 2:OF:205:LEU:CB | 2.93                     | 0.47              |
| 3:PF:301:VAL:O   | 3:PF:321:ILE:N  | 2.45                     | 0.47              |
| 2:UF:119:ALA:O   | 2:UF:123:ARG:N  | 2.44                     | 0.47              |
| 3:VF:301:VAL:O   | 3:VF:321:ILE:N  | 2.45                     | 0.47              |
| 2:GG:139:ARG:C   | 2:MG:205:LEU:CB | 2.88                     | 0.47              |
| 4:KG:100:LEU:HA  | 4:KG:105:LEU:HA | 1.96                     | 0.47              |
| 2:MG:119:ALA:O   | 2:MG:123:ARG:N  | 2.44                     | 0.47              |
| 4:R:110:GLU:O    | 4:R:121:ARG:N   | 2.42                     | 0.47              |
| 2:GA:139:ARG:O   | 2:MA:205:LEU:CB | 2.63                     | 0.47              |
| 3:LB:80:THR:O    | 3:LB:205:HIS:N  | 2.35                     | 0.47              |
| 2:IC:139:ARG:CB  | 2:OC:205:LEU:CB | 2.93                     | 0.47              |
| 2:MD:77:LEU:CB   | 2:SD:42:ALA:C   | 2.88                     | 0.47              |
| 3:DF:80:THR:O    | 3:DF:205:HIS:N  | 2.35                     | 0.47              |
| 3:NG:80:THR:O    | 3:NG:205:HIS:N  | 2.35                     | 0.47              |
| 3:TG:301:VAL:O   | 3:TG:321:ILE:N  | 2.45                     | 0.47              |
| 2:SA:139:ARG:C   | 2:YA:205:LEU:CB | 2.88                     | 0.47              |
| 4:SF:100:LEU:HA  | 4:SF:105:LEU:HA | 1.96                     | 0.47              |
| 4:YF:110:GLU:O   | 4:YF:121:ARG:N  | 2.42                     | 0.47              |
| 3:BG:301:VAL:O   | 3:BG:321:ILE:N  | 2.45                     | 0.47              |
| 3:NG:301:VAL:O   | 3:NG:321:ILE:N  | 2.45                     | 0.47              |
| 3:M:80:THR:O     | 3:M:205:HIS:N   | 2.35                     | 0.47              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:VC:80:THR:O    | 3:VC:205:HIS:N  | 2.35                     | 0.47              |
| 2:SD:139:ARG:C   | 2:YD:205:LEU:CB | 2.89                     | 0.47              |
| 2:QE:139:ARG:C   | 2:WE:205:LEU:CB | 2.87                     | 0.47              |
| 4:YF:100:LEU:HA  | 4:YF:105:LEU:HA | 1.96                     | 0.47              |
| 3:HG:301:VAL:O   | 3:HG:321:ILE:N  | 2.45                     | 0.47              |
| 4:H:110:GLU:O    | 4:H:121:ARG:N   | 2.42                     | 0.46              |
| 4:CE:100:LEU:HA  | 4:CE:105:LEU:HA | 1.96                     | 0.46              |
| 2:CF:139:ARG:C   | 2:IF:205:LEU:CB | 2.88                     | 0.46              |
| 4:SF:110:GLU:O   | 4:SF:121:ARG:N  | 2.42                     | 0.46              |
| 2:UF:139:ARG:C   | 2:AG:205:LEU:CB | 2.88                     | 0.46              |
| 4:EG:100:LEU:HA  | 4:EG:105:LEU:HA | 1.96                     | 0.46              |
| 4:Q:110:GLU:O    | 4:Q:121:ARG:N   | 2.42                     | 0.46              |
| 3:FB:270:LEU:O   | 4:GB:62:VAL:N   | 2.27                     | 0.46              |
| 4:WD:100:LEU:HA  | 4:WD:105:LEU:HA | 1.96                     | 0.46              |
| 4:IE:100:LEU:HA  | 4:IE:105:LEU:HA | 1.96                     | 0.46              |
| 4:MF:100:LEU:HA  | 4:MF:105:LEU:HA | 1.96                     | 0.46              |
| 2:SD:119:ALA:O   | 2:SD:123:ARG:N  | 2.44                     | 0.46              |
| 4:AF:100:LEU:HA  | 4:AF:105:LEU:HA | 1.96                     | 0.46              |
| 4:MF:110:GLU:O   | 4:MF:121:ARG:N  | 2.42                     | 0.46              |
| 4:GF:100:LEU:HA  | 4:GF:105:LEU:HA | 1.96                     | 0.46              |
| 4:OE:100:LEU:HA  | 4:OE:105:LEU:HA | 1.96                     | 0.46              |
| 4:UE:100:LEU:HA  | 4:UE:105:LEU:HA | 1.96                     | 0.46              |
| 4:GF:110:GLU:O   | 4:GF:121:ARG:N  | 2.42                     | 0.46              |
| 3:JF:80:THR:O    | 3:JF:205:HIS:N  | 2.35                     | 0.46              |
| 3:HA:80:THR:O    | 3:HA:205:HIS:N  | 2.35                     | 0.46              |
| 3:TG:80:THR:O    | 3:TG:205:HIS:N  | 2.35                     | 0.46              |
| 4:AF:110:GLU:O   | 4:AF:121:ARG:N  | 2.42                     | 0.46              |
| 2:UF:200:ALA:HB3 | 2:UF:232:GLU:CB | 2.32                     | 0.46              |
| 2:OC:147:ALA:HA  | 2:UC:210:GLN:CB | 2.46                     | 0.45              |
| 3:BG:80:THR:O    | 3:BG:205:HIS:N  | 2.35                     | 0.45              |
| 4:WG:110:GLU:O   | 4:WG:121:ARG:N  | 2.42                     | 0.45              |
| 2:KE:139:ARG:CB  | 2:QE:205:LEU:CB | 2.94                     | 0.45              |
| 4:YF:106:ILE:O   | 4:YF:126:ILE:N  | 2.40                     | 0.45              |
| 2:T:139:ARG:O    | 2:AA:205:LEU:CB | 2.64                     | 0.45              |
| 2:CC:139:ARG:C   | 2:IC:205:LEU:CB | 2.90                     | 0.45              |
| 4:UE:110:GLU:O   | 4:UE:121:ARG:N  | 2.42                     | 0.45              |
| 4:QG:110:GLU:O   | 4:QG:121:ARG:N  | 2.42                     | 0.45              |
| 4:CB:106:ILE:O   | 4:CB:126:ILE:N  | 2.40                     | 0.45              |
| 2:EE:139:ARG:C   | 2:KE:205:LEU:CB | 2.90                     | 0.45              |
| 3:PF:80:THR:O    | 3:PF:205:HIS:N  | 2.35                     | 0.45              |
| 2:G:139:ARG:C    | 2:B:205:LEU:CB  | 2.90                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:EB:139:ARG:O   | 2:KB:205:LEU:CB | 2.65                     | 0.45              |
| 3:RB:80:THR:O    | 3:RB:205:HIS:N  | 2.35                     | 0.45              |
| 2:OF:139:ARG:O   | 2:UF:205:LEU:CB | 2.64                     | 0.45              |
| 4:EG:106:ILE:O   | 4:EG:126:ILE:N  | 2.40                     | 0.45              |
| 2:G:205:LEU:CB   | 2:SG:139:ARG:O  | 2.64                     | 0.44              |
| 4:OE:110:GLU:O   | 4:OE:121:ARG:N  | 2.42                     | 0.44              |
| 4:KG:110:GLU:O   | 4:KG:121:ARG:N  | 2.42                     | 0.44              |
| 4:ED:106:ILE:O   | 4:ED:126:ILE:N  | 2.40                     | 0.44              |
| 2:J:139:ARG:CB   | 2:T:205:LEU:CB  | 2.95                     | 0.44              |
| 2:MA:77:LEU:CB   | 2:SA:42:ALA:C   | 2.90                     | 0.44              |
| 2:WB:139:ARG:O   | 2:CC:205:LEU:CB | 2.65                     | 0.44              |
| 2:MD:139:ARG:C   | 2:SD:205:LEU:CB | 2.91                     | 0.44              |
| 4:KG:106:ILE:O   | 4:KG:126:ILE:N  | 2.40                     | 0.44              |
| 2:OC:200:ALA:HB3 | 2:OC:232:GLU:CB | 2.32                     | 0.44              |
| 4:SC:110:GLU:O   | 4:SC:121:ARG:N  | 2.42                     | 0.44              |
| 3:BD:80:THR:O    | 3:BD:205:HIS:N  | 2.35                     | 0.44              |
| 4:PD:120:VAL:N   | 4:QD:87:VAL:O   | 2.51                     | 0.44              |
| 2:SD:200:ALA:HB3 | 2:SD:232:GLU:CB | 2.32                     | 0.44              |
| 4:NE:120:VAL:N   | 4:OE:87:VAL:O   | 2.51                     | 0.44              |
| 2:MG:139:ARG:C   | 2:SG:205:LEU:CB | 2.91                     | 0.44              |
| 4:O:120:VAL:N    | 4:R:87:VAL:O    | 2.51                     | 0.44              |
| 2:KB:200:ALA:HB3 | 2:KB:232:GLU:CB | 2.32                     | 0.44              |
| 2:WB:139:ARG:CB  | 2:CC:205:LEU:CB | 2.95                     | 0.44              |
| 4:JD:120:VAL:N   | 4:KD:87:VAL:O   | 2.51                     | 0.44              |
| 4:IE:110:GLU:O   | 4:IE:121:ARG:N  | 2.42                     | 0.44              |
| 4:PG:120:VAL:N   | 4:QG:87:VAL:O   | 2.51                     | 0.44              |
| 2:G:200:ALA:HB3  | 2:G:232:GLU:CB  | 2.32                     | 0.44              |
| 4:X:120:VAL:N    | 4:Y:87:VAL:O    | 2.51                     | 0.44              |
| 2:IC:139:ARG:O   | 2:OC:205:LEU:CB | 2.66                     | 0.44              |
| 2:AG:139:ARG:O   | 2:GG:205:LEU:CB | 2.65                     | 0.44              |
| 4:EG:110:GLU:O   | 4:EG:121:ARG:N  | 2.42                     | 0.44              |
| 2:YA:139:ARG:O   | 2:EB:205:LEU:CB | 2.66                     | 0.44              |
| 4:RF:120:VAL:N   | 4:SF:87:VAL:O   | 2.51                     | 0.44              |
| 2:GA:200:ALA:HB3 | 2:GA:232:GLU:CB | 2.32                     | 0.44              |
| 4:BB:120:VAL:N   | 4:CB:87:VAL:O   | 2.51                     | 0.44              |
| 2:QB:139:ARG:C   | 2:WB:205:LEU:CB | 2.91                     | 0.44              |
| 4:HE:120:VAL:N   | 4:IE:87:VAL:O   | 2.51                     | 0.44              |
| 4:TE:120:VAL:N   | 4:UE:87:VAL:O   | 2.51                     | 0.44              |
| 2:WE:139:ARG:C   | 2:CF:205:LEU:CB | 2.90                     | 0.44              |
| 4:LF:120:VAL:N   | 4:MF:87:VAL:O   | 2.51                     | 0.44              |
| 4:JG:120:VAL:N   | 4:KG:87:VAL:O   | 2.51                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:VG:120:VAL:N   | 4:WG:87:VAL:O   | 2.51                     | 0.44              |
| 4:VA:120:VAL:N   | 4:WA:87:VAL:O   | 2.51                     | 0.43              |
| 4:FC:120:VAL:N   | 4:GC:87:VAL:O   | 2.51                     | 0.43              |
| 4:LC:120:VAL:N   | 4:MC:87:VAL:O   | 2.51                     | 0.43              |
| 4:CE:110:GLU:O   | 4:CE:121:ARG:N  | 2.42                     | 0.43              |
| 3:FE:80:THR:O    | 3:FE:205:HIS:N  | 2.35                     | 0.43              |
| 4:DG:120:VAL:N   | 4:EG:87:VAL:O   | 2.51                     | 0.43              |
| 4:DA:120:VAL:N   | 4:EA:87:VAL:O   | 2.51                     | 0.43              |
| 4:VD:120:VAL:N   | 4:WD:87:VAL:O   | 2.51                     | 0.43              |
| 2:KE:190:ARG:O   | 2:KE:191:SER:C  | 2.61                     | 0.43              |
| 3:VF:80:THR:O    | 3:VF:205:HIS:N  | 2.35                     | 0.43              |
| 2:G:205:LEU:CB   | 2:SG:139:ARG:CB | 2.96                     | 0.43              |
| 3:C:80:THR:O     | 3:C:205:HIS:N   | 2.35                     | 0.43              |
| 4:E:120:VAL:N    | 4:H:87:VAL:O    | 2.51                     | 0.43              |
| 4:HB:120:VAL:N   | 4:IB:87:VAL:O   | 2.51                     | 0.43              |
| 4:DD:120:VAL:N   | 4:ED:87:VAL:O   | 2.51                     | 0.43              |
| 2:EE:190:ARG:O   | 2:EE:191:SER:C  | 2.62                     | 0.43              |
| 2:KE:147:ALA:HA  | 2:QE:210:GLN:CB | 2.48                     | 0.43              |
| 2:QE:190:ARG:O   | 2:QE:191:SER:C  | 2.61                     | 0.43              |
| 2:WE:200:ALA:HB3 | 2:WE:232:GLU:CB | 2.32                     | 0.43              |
| 4:QG:106:ILE:O   | 4:QG:126:ILE:N  | 2.40                     | 0.43              |
| 4:PA:120:VAL:N   | 4:QA:87:VAL:O   | 2.51                     | 0.43              |
| 4:IB:106:ILE:O   | 4:IB:126:ILE:N  | 2.40                     | 0.43              |
| 4:ZB:120:VAL:N   | 4:AC:87:VAL:O   | 2.51                     | 0.43              |
| 2:GD:139:ARG:O   | 2:MD:205:LEU:CB | 2.67                     | 0.43              |
| 2:YD:139:ARG:O   | 2:EE:205:LEU:CB | 2.66                     | 0.43              |
| 2:WE:190:ARG:O   | 2:WE:191:SER:C  | 2.61                     | 0.43              |
| 4:RC:120:VAL:N   | 4:SC:87:VAL:O   | 2.51                     | 0.43              |
| 2:SD:139:ARG:CB  | 2:YD:205:LEU:CB | 2.97                     | 0.43              |
| 2:QE:139:ARG:O   | 2:WE:205:LEU:CB | 2.66                     | 0.43              |
| 2:CF:190:ARG:O   | 2:CF:191:SER:C  | 2.61                     | 0.43              |
| 4:FF:120:VAL:N   | 4:GF:87:VAL:O   | 2.51                     | 0.43              |
| 4:XF:120:VAL:N   | 4:YF:87:VAL:O   | 2.51                     | 0.43              |
| 4:KD:106:ILE:O   | 4:KD:126:ILE:N  | 2.40                     | 0.43              |
| 4:WD:110:GLU:O   | 4:WD:121:ARG:N  | 2.42                     | 0.43              |
| 2:IF:190:ARG:O   | 2:IF:191:SER:C  | 2.61                     | 0.43              |
| 2:OF:188:LEU:O   | 2:OF:189:LYS:C  | 2.62                     | 0.43              |
| 2:J:139:ARG:O    | 2:T:205:LEU:CB  | 2.66                     | 0.43              |
| 4:ZE:120:VAL:N   | 4:AF:87:VAL:O   | 2.51                     | 0.43              |
| 2:IF:188:LEU:O   | 2:IF:189:LYS:C  | 2.62                     | 0.43              |
| 2:UF:188:LEU:O   | 2:UF:189:LYS:C  | 2.62                     | 0.43              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:AG:188:LEU:O  | 2:AG:189:LYS:C  | 2.62                     | 0.43              |
| 2:GG:188:LEU:O  | 2:GG:189:LYS:C  | 2.62                     | 0.43              |
| 4:P:120:VAL:N   | 4:Q:87:VAL:O    | 2.51                     | 0.43              |
| 3:NA:80:THR:O   | 3:NA:205:HIS:N  | 2.35                     | 0.43              |
| 4:BE:120:VAL:N  | 4:CE:87:VAL:O   | 2.51                     | 0.43              |
| 2:CF:188:LEU:O  | 2:CF:189:LYS:C  | 2.62                     | 0.43              |
| 2:MG:188:LEU:O  | 2:MG:189:LYS:C  | 2.62                     | 0.43              |
| 2:SG:188:LEU:O  | 2:SG:189:LYS:C  | 2.62                     | 0.43              |
| 2:B:139:ARG:O   | 2:J:205:LEU:CB  | 2.66                     | 0.43              |
| 2:OF:190:ARG:O  | 2:OF:191:SER:C  | 2.61                     | 0.43              |
| 2:SA:139:ARG:O  | 2:YA:205:LEU:CB | 2.67                     | 0.43              |
| 2:EB:139:ARG:CB | 2:KB:205:LEU:CB | 2.97                     | 0.43              |
| 4:NB:120:VAL:N  | 4:OB:87:VAL:O   | 2.51                     | 0.43              |
| 2:UF:190:ARG:O  | 2:UF:191:SER:C  | 2.61                     | 0.43              |
| 4:WG:106:ILE:O  | 4:WG:126:ILE:N  | 2.40                     | 0.43              |
| 2:G:188:LEU:O   | 2:G:189:LYS:C   | 2.62                     | 0.42              |
| 4:JA:120:VAL:N  | 4:KA:87:VAL:O   | 2.51                     | 0.42              |
| 2:OC:73:ALA:HA  | 2:UC:43:ASN:HA  | 2.00                     | 0.42              |
| 3:HD:80:THR:O   | 3:HD:205:HIS:N  | 2.35                     | 0.42              |
| 3:ND:80:THR:O   | 3:ND:205:HIS:N  | 2.35                     | 0.42              |
| 4:QD:110:GLU:O  | 4:QD:121:ARG:N  | 2.42                     | 0.42              |
| 2:B:188:LEU:O   | 2:B:189:LYS:C   | 2.62                     | 0.42              |
| 2:MA:190:ARG:O  | 2:MA:191:SER:C  | 2.61                     | 0.42              |
| 2:UC:139:ARG:C  | 2:AD:205:LEU:CB | 2.92                     | 0.42              |
| 4:XC:120:VAL:N  | 4:YC:87:VAL:O   | 2.51                     | 0.42              |
| 2:AD:139:ARG:CB | 2:GD:205:LEU:CB | 2.97                     | 0.42              |
| 2:AG:190:ARG:O  | 2:AG:191:SER:C  | 2.61                     | 0.42              |
| 2:AA:139:ARG:CB | 2:GA:205:LEU:CB | 2.97                     | 0.42              |
| 2:GA:190:ARG:O  | 2:GA:191:SER:C  | 2.61                     | 0.42              |
| 2:SA:190:ARG:O  | 2:SA:191:SER:C  | 2.61                     | 0.42              |
| 3:BD:80:THR:N   | 3:BD:205:HIS:O  | 2.33                     | 0.42              |
| 3:TD:80:THR:O   | 3:TD:205:HIS:N  | 2.35                     | 0.42              |
| 2:J:188:LEU:O   | 2:J:189:LYS:C   | 2.62                     | 0.42              |
| 2:AA:139:ARG:O  | 2:GA:205:LEU:CB | 2.67                     | 0.42              |
| 2:AA:190:ARG:O  | 2:AA:191:SER:C  | 2.61                     | 0.42              |
| 3:XB:80:THR:O   | 3:XB:205:HIS:N  | 2.35                     | 0.42              |
| 2:GA:139:ARG:CB | 2:MA:205:LEU:CB | 2.97                     | 0.42              |
| 2:YA:190:ARG:O  | 2:YA:191:SER:C  | 2.61                     | 0.42              |
| 4:QC:65:THR:N   | 4:QC:100:LEU:O  | 2.40                     | 0.42              |
| 2:EE:139:ARG:CB | 2:KE:205:LEU:CB | 2.97                     | 0.42              |
| 2:GG:190:ARG:O  | 2:GG:191:SER:C  | 2.61                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:K:80:THR:O     | 3:K:205:HIS:N   | 2.35                     | 0.42              |
| 2:T:188:LEU:O    | 2:T:189:LYS:C   | 2.62                     | 0.42              |
| 2:T:190:ARG:O    | 2:T:191:SER:C   | 2.61                     | 0.42              |
| 4:WC:65:THR:N    | 4:WC:100:LEU:O  | 2.40                     | 0.42              |
| 4:KD:110:GLU:O   | 4:KD:121:ARG:N  | 2.42                     | 0.42              |
| 2:KB:188:LEU:O   | 2:KB:189:LYS:C  | 2.62                     | 0.42              |
| 4:KC:65:THR:N    | 4:KC:100:LEU:O  | 2.40                     | 0.42              |
| 3:PC:80:THR:O    | 3:PC:205:HIS:N  | 2.35                     | 0.42              |
| 3:ZD:80:THR:O    | 3:ZD:205:HIS:N  | 2.35                     | 0.42              |
| 2:MG:190:ARG:O   | 2:MG:191:SER:C  | 2.61                     | 0.42              |
| 2:AA:188:LEU:O   | 2:AA:189:LYS:C  | 2.62                     | 0.42              |
| 3:TA:80:THR:O    | 3:TA:205:HIS:N  | 2.35                     | 0.42              |
| 2:EB:188:LEU:O   | 2:EB:189:LYS:C  | 2.62                     | 0.42              |
| 2:EB:190:ARG:O   | 2:EB:191:SER:C  | 2.61                     | 0.42              |
| 2:KB:147:ALA:HA  | 2:QB:210:GLN:CB | 2.49                     | 0.42              |
| 2:QB:188:LEU:O   | 2:QB:189:LYS:C  | 2.62                     | 0.42              |
| 4:CD:65:THR:N    | 4:CD:100:LEU:O  | 2.40                     | 0.42              |
| 2:KE:73:ALA:HA   | 2:QE:43:ASN:HA  | 2.00                     | 0.42              |
| 2:GG:139:ARG:O   | 2:MG:205:LEU:CB | 2.67                     | 0.42              |
| 4:Q:106:ILE:O    | 4:Q:126:ILE:N   | 2.40                     | 0.42              |
| 2:SA:139:ARG:CB  | 2:YA:205:LEU:CB | 2.97                     | 0.42              |
| 2:KB:190:ARG:O   | 2:KB:191:SER:C  | 2.61                     | 0.42              |
| 4:TB:120:VAL:N   | 4:UB:87:VAL:O   | 2.51                     | 0.42              |
| 2:WB:188:LEU:O   | 2:WB:189:LYS:C  | 2.62                     | 0.42              |
| 2:IC:190:ARG:O   | 2:IC:191:SER:C  | 2.61                     | 0.42              |
| 2:MD:200:ALA:HB3 | 2:MD:232:GLU:CB | 2.32                     | 0.42              |
| 4:QD:106:ILE:O   | 4:QD:126:ILE:N  | 2.40                     | 0.42              |
| 3:HG:80:THR:O    | 3:HG:205:HIS:N  | 2.35                     | 0.42              |
| 2:J:190:ARG:O    | 2:J:191:SER:C   | 2.61                     | 0.42              |
| 2:GA:188:LEU:O   | 2:GA:189:LYS:C  | 2.62                     | 0.42              |
| 2:YA:188:LEU:O   | 2:YA:189:LYS:C  | 2.62                     | 0.42              |
| 4:OB:106:ILE:O   | 4:OB:126:ILE:N  | 2.40                     | 0.42              |
| 2:CC:188:LEU:O   | 2:CC:189:LYS:C  | 2.62                     | 0.42              |
| 2:CC:190:ARG:O   | 2:CC:191:SER:C  | 2.61                     | 0.42              |
| 2:IC:200:ALA:HB3 | 2:IC:232:GLU:CB | 2.32                     | 0.42              |
| 3:JC:80:THR:O    | 3:JC:205:HIS:N  | 2.35                     | 0.42              |
| 2:OC:190:ARG:O   | 2:OC:191:SER:C  | 2.61                     | 0.42              |
| 4:ED:110:GLU:O   | 4:ED:121:ARG:N  | 2.42                     | 0.42              |
| 2:SG:190:ARG:O   | 2:SG:191:SER:C  | 2.61                     | 0.42              |
| 2:OC:188:LEU:O   | 2:OC:189:LYS:C  | 2.62                     | 0.41              |
| 2:AD:188:LEU:O   | 2:AD:189:LYS:C  | 2.62                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:GD:188:LEU:O   | 2:GD:189:LYS:C  | 2.62                     | 0.41              |
| 2:SD:139:ARG:O   | 2:YD:205:LEU:CB | 2.68                     | 0.41              |
| 2:CF:139:ARG:CB  | 2:IF:205:LEU:CB | 2.98                     | 0.41              |
| 2:AG:139:ARG:CB  | 2:GG:205:LEU:CB | 2.98                     | 0.41              |
| 2:AG:200:ALA:HB3 | 2:AG:232:GLU:CB | 2.32                     | 0.41              |
| 2:T:139:ARG:CB   | 2:AA:205:LEU:CB | 2.98                     | 0.41              |
| 2:MA:139:ARG:C   | 2:SA:205:LEU:CB | 2.93                     | 0.41              |
| 2:MA:188:LEU:O   | 2:MA:189:LYS:C  | 2.62                     | 0.41              |
| 2:SA:188:LEU:O   | 2:SA:189:LYS:C  | 2.62                     | 0.41              |
| 3:ZA:80:THR:O    | 3:ZA:205:HIS:N  | 2.35                     | 0.41              |
| 2:WB:190:ARG:O   | 2:WB:191:SER:C  | 2.61                     | 0.41              |
| 4:EC:65:THR:N    | 4:EC:100:LEU:O  | 2.40                     | 0.41              |
| 2:IC:188:LEU:O   | 2:IC:189:LYS:C  | 2.62                     | 0.41              |
| 2:UC:188:LEU:O   | 2:UC:189:LYS:C  | 2.62                     | 0.41              |
| 2:UC:190:ARG:O   | 2:UC:191:SER:C  | 2.61                     | 0.41              |
| 4:ID:65:THR:N    | 4:ID:100:LEU:O  | 2.40                     | 0.41              |
| 2:MD:188:LEU:O   | 2:MD:189:LYS:C  | 2.62                     | 0.41              |
| 2:G:190:ARG:O    | 2:G:191:SER:C   | 2.61                     | 0.41              |
| 3:LB:80:THR:N    | 3:LB:205:HIS:O  | 2.33                     | 0.41              |
| 2:QB:190:ARG:O   | 2:QB:191:SER:C  | 2.61                     | 0.41              |
| 2:CC:139:ARG:CB  | 2:IC:205:LEU:CB | 2.99                     | 0.41              |
| 3:DC:80:THR:O    | 3:DC:205:HIS:N  | 2.35                     | 0.41              |
| 4:YC:110:GLU:O   | 4:YC:121:ARG:N  | 2.42                     | 0.41              |
| 2:MD:139:ARG:O   | 2:SD:205:LEU:CB | 2.68                     | 0.41              |
| 3:LE:80:THR:N    | 3:LE:205:HIS:O  | 2.33                     | 0.41              |
| 2:UF:139:ARG:O   | 2:AG:205:LEU:CB | 2.67                     | 0.41              |
| 2:OC:139:ARG:CB  | 2:UC:205:LEU:CB | 2.99                     | 0.41              |
| 2:AD:190:ARG:O   | 2:AD:191:SER:C  | 2.61                     | 0.41              |
| 2:SD:188:LEU:O   | 2:SD:189:LYS:C  | 2.62                     | 0.41              |
| 2:YD:188:LEU:O   | 2:YD:189:LYS:C  | 2.62                     | 0.41              |
| 2:IF:139:ARG:O   | 2:OF:205:LEU:CB | 2.67                     | 0.41              |
| 2:MG:139:ARG:CB  | 2:SG:205:LEU:CB | 2.98                     | 0.41              |
| 2:B:139:ARG:CB   | 2:J:205:LEU:CB  | 2.98                     | 0.41              |
| 2:B:190:ARG:O    | 2:B:191:SER:C   | 2.61                     | 0.41              |
| 4:KA:106:ILE:O   | 4:KA:126:ILE:N  | 2.40                     | 0.41              |
| 3:DC:85:ARG:O    | 3:DC:201:ASN:N  | 2.34                     | 0.41              |
| 2:GD:139:ARG:CB  | 2:MD:205:LEU:CB | 2.99                     | 0.41              |
| 2:CF:139:ARG:O   | 2:IF:205:LEU:CB | 2.67                     | 0.41              |
| 4:QA:106:ILE:O   | 4:QA:126:ILE:N  | 2.40                     | 0.41              |
| 2:AD:147:ALA:HA  | 2:GD:210:GLN:CB | 2.50                     | 0.41              |
| 4:WA:106:ILE:O   | 4:WA:126:ILE:N  | 2.40                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:YB:65:THR:N   | 4:YB:100:LEU:O  | 2.40                     | 0.41              |
| 2:GD:190:ARG:O  | 2:GD:191:SER:C  | 2.61                     | 0.41              |
| 2:EE:188:LEU:O  | 2:EE:189:LYS:C  | 2.62                     | 0.41              |
| 3:VC:80:THR:N   | 3:VC:205:HIS:O  | 2.33                     | 0.41              |
| 4:OD:65:THR:N   | 4:OD:100:LEU:O  | 2.40                     | 0.41              |
| 2:KE:188:LEU:O  | 2:KE:189:LYS:C  | 2.62                     | 0.41              |
| 2:OF:139:ARG:CB | 2:UF:205:LEU:CB | 2.99                     | 0.41              |
| 4:QF:64:LEU:HA  | 4:QF:101:ILE:HA | 2.03                     | 0.41              |
| 4:CG:64:LEU:HA  | 4:CG:101:ILE:HA | 2.03                     | 0.41              |
| 4:N:64:LEU:HA   | 4:N:101:ILE:HA  | 2.03                     | 0.41              |
| 4:H:106:ILE:O   | 4:H:126:ILE:N   | 2.40                     | 0.41              |
| 4:L:64:LEU:HA   | 4:L:101:ILE:HA  | 2.03                     | 0.41              |
| 3:V:80:THR:O    | 3:V:205:HIS:N   | 2.35                     | 0.41              |
| 3:FB:80:THR:N   | 3:FB:205:HIS:O  | 2.33                     | 0.41              |
| 2:QB:139:ARG:CB | 2:WB:205:LEU:CB | 2.99                     | 0.41              |
| 4:XC:106:ILE:O  | 4:XC:126:ILE:HA | 2.21                     | 0.41              |
| 4:BE:106:ILE:O  | 4:BE:126:ILE:HA | 2.21                     | 0.41              |
| 4:HE:106:ILE:O  | 4:HE:126:ILE:HA | 2.21                     | 0.41              |
| 2:QE:188:LEU:O  | 2:QE:189:LYS:C  | 2.62                     | 0.41              |
| 4:SE:64:LEU:HA  | 4:SE:101:ILE:HA | 2.03                     | 0.41              |
| 4:UE:106:ILE:O  | 4:UE:126:ILE:N  | 2.40                     | 0.41              |
| 4:EF:64:LEU:HA  | 4:EF:101:ILE:HA | 2.03                     | 0.41              |
| 4:KF:64:LEU:HA  | 4:KF:101:ILE:HA | 2.03                     | 0.41              |
| 4:LF:106:ILE:O  | 4:LF:126:ILE:HA | 2.21                     | 0.41              |
| 4:WF:64:LEU:HA  | 4:WF:101:ILE:HA | 2.03                     | 0.41              |
| 4:OG:64:LEU:HA  | 4:OG:101:ILE:HA | 2.03                     | 0.41              |
| 4:D:64:LEU:HA   | 4:D:101:ILE:HA  | 2.03                     | 0.41              |
| 2:MD:190:ARG:O  | 2:MD:191:SER:C  | 2.61                     | 0.41              |
| 4:GE:64:LEU:HA  | 4:GE:101:ILE:HA | 2.03                     | 0.41              |
| 3:LE:80:THR:O   | 3:LE:205:HIS:N  | 2.35                     | 0.41              |
| 4:FF:106:ILE:O  | 4:FF:126:ILE:HA | 2.21                     | 0.41              |
| 4:CA:64:LEU:HA  | 4:CA:101:ILE:HA | 2.03                     | 0.40              |
| 2:GA:147:ALA:HA | 2:MA:210:GLN:CB | 2.51                     | 0.40              |
| 2:AD:73:ALA:HA  | 2:GD:43:ASN:HA  | 2.03                     | 0.40              |
| 4:DD:106:ILE:O  | 4:DD:126:ILE:HA | 2.21                     | 0.40              |
| 4:WD:106:ILE:O  | 4:WD:126:ILE:N  | 2.40                     | 0.40              |
| 4:ME:64:LEU:HA  | 4:ME:101:ILE:HA | 2.03                     | 0.40              |
| 4:YE:64:LEU:HA  | 4:YE:101:ILE:HA | 2.03                     | 0.40              |
| 4:IG:64:LEU:HA  | 4:IG:101:ILE:HA | 2.03                     | 0.40              |
| 4:UG:64:LEU:HA  | 4:UG:101:ILE:HA | 2.03                     | 0.40              |
| 2:G:139:ARG:O   | 2:B:205:LEU:CB  | 2.69                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:O:106:ILE:O    | 4:O:126:ILE:HA  | 2.21                     | 0.40              |
| 4:PA:106:ILE:O   | 4:PA:126:ILE:HA | 2.21                     | 0.40              |
| 2:QB:200:ALA:HB3 | 2:QB:232:GLU:CB | 2.32                     | 0.40              |
| 2:CC:139:ARG:O   | 2:IC:205:LEU:CB | 2.69                     | 0.40              |
| 4:RC:106:ILE:O   | 4:RC:126:ILE:HA | 2.21                     | 0.40              |
| 2:UC:200:ALA:HB3 | 2:UC:232:GLU:CB | 2.32                     | 0.40              |
| 2:QE:139:ARG:CB  | 2:WE:205:LEU:CB | 2.99                     | 0.40              |
| 2:WE:139:ARG:O   | 2:CF:205:LEU:CB | 2.68                     | 0.40              |
| 4:VG:106:ILE:O   | 4:VG:126:ILE:HA | 2.21                     | 0.40              |
| 4:X:106:ILE:O    | 4:X:126:ILE:HA  | 2.21                     | 0.40              |
| 4:SB:65:THR:N    | 4:SB:100:LEU:O  | 2.40                     | 0.40              |
| 4:TB:106:ILE:O   | 4:TB:126:ILE:HA | 2.21                     | 0.40              |
| 4:VD:106:ILE:O   | 4:VD:126:ILE:HA | 2.21                     | 0.40              |
| 2:YD:200:ALA:HB3 | 2:YD:232:GLU:CB | 2.32                     | 0.40              |
| 4:NE:106:ILE:O   | 4:NE:126:ILE:HA | 2.21                     | 0.40              |
| 2:WE:188:LEU:O   | 2:WE:189:LYS:C  | 2.62                     | 0.40              |
| 4:RF:106:ILE:O   | 4:RF:126:ILE:HA | 2.21                     | 0.40              |
| 4:OA:64:LEU:HA   | 4:OA:101:ILE:HA | 2.03                     | 0.40              |
| 3:ZA:80:THR:N    | 3:ZA:205:HIS:O  | 2.33                     | 0.40              |
| 4:ZB:106:ILE:O   | 4:ZB:126:ILE:HA | 2.21                     | 0.40              |
| 4:AE:64:LEU:HA   | 4:AE:101:ILE:HA | 2.03                     | 0.40              |
| 2:EE:139:ARG:O   | 2:KE:205:LEU:CB | 2.70                     | 0.40              |
| 2:B:200:ALA:HB3  | 2:B:232:GLU:CB  | 2.32                     | 0.40              |
| 4:W:64:LEU:HA    | 4:W:101:ILE:HA  | 2.03                     | 0.40              |
| 4:UB:106:ILE:O   | 4:UB:126:ILE:N  | 2.40                     | 0.40              |
| 4:OD:64:LEU:HA   | 4:OD:101:ILE:HA | 2.03                     | 0.40              |
| 4:UD:64:LEU:HA   | 4:UD:101:ILE:HA | 2.03                     | 0.40              |
| 4:UD:65:THR:N    | 4:UD:100:LEU:O  | 2.40                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | BC    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | BF    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | DB    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | DE    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | F     | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | FA    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | FD    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | FG    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | HC    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | HF    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | I     | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | JB    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | JE    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | LA    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | LD    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | LG    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | NC    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | NF    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | PB    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | PE    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | RA    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | RD    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | RG    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | S     | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | TC    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | TF    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | VB    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | VE    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | XA    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | XD    | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | Z     | 45/560 (8%) | 44 (98%) | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | ZC    | 45/560 (8%)   | 44 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | ZF    | 45/560 (8%)   | 44 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 2   | AA    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | AD    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | AG    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | B     | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | CC    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | CF    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | EB    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | EE    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | G     | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | GA    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | GD    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | GG    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | IC    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | IF    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | J     | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | KB    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | KE    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | MA    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | MD    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | MG    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | OC    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | OF    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | QB    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | QE    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | SA    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | SD    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | SG    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | T     | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | UC    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | UF    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | WB    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | WE    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | YA    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 2   | YD    | 315/331 (95%) | 299 (95%) | 15 (5%) | 1 (0%)   | 36          | 72  |
| 3   | BA    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | BD    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | BG    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | C     | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | DC    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | DF    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | FB    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | FE    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | HA    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | HD    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | HG    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | JC    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | JF    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | K     | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | LB    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | LE    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | M     | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | NA    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | ND    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | NG    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | PC    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | PF    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | RB    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | RE    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | TA    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | TD    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | TG    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | V     | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | VC    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | VF    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | XB    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | XE    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | ZA    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | ZD    | 285/334 (85%) | 274 (96%) | 11 (4%) | 0        | 100         | 100 |
| 4   | AB    | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | AC    | 79/137 (58%)  | 74 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 4   | AE    | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | AF    | 79/137 (58%)  | 74 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 4   | BB    | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |
| 4   | BE    | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |
| 4   | CA    | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | CB    | 79/137 (58%)  | 74 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 4   | CD    | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | CE    | 79/137 (58%)  | 74 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 4   | CG    | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | D     | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | DA    | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |
| 4   | DD    | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |
| 4   | DG    | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |
| 4   | E     | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |
| 4   | EA    | 79/137 (58%)  | 74 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 4   | EC    | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | ED    | 79/137 (58%)  | 74 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 4   | EF    | 91/137 (66%)  | 88 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | EG    | 79/137 (58%)  | 74 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 4   | FC    | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |
| 4   | FF    | 81/137 (59%)  | 73 (90%)  | 8 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|--------------|----------|---------|----------|-------------|-----|
| 4   | GB    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | GC    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | GE    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | GF    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | H     | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | HB    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | HE    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | IA    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | IB    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | ID    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | IE    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | IG    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | JA    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | JD    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | JG    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | KA    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | KC    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | KD    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | KF    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | KG    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | L     | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | LC    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | LF    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | MB    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | MC    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | ME    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | MF    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | N     | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | NB    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | NE    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | O     | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|--------------|----------|---------|----------|-------------|-----|
| 4   | OA    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | OB    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | OD    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | OE    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | OG    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | P     | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | PA    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | PD    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | PG    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | Q     | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | QA    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | QC    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | QD    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | QF    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | QG    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | R     | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | RC    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | RF    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | SB    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | SC    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | SE    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | SF    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | TB    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | TE    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | UA    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | UB    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | UD    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | UE    | 79/137 (58%) | 74 (94%) | 5 (6%)  | 0        | 100         | 100 |
| 4   | UG    | 91/137 (66%) | 88 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 4   | VA    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |
| 4   | VD    | 81/137 (59%) | 73 (90%) | 8 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 4   | VG    | 81/137 (59%)      | 73 (90%)    | 8 (10%)   | 0        | 100         | 100 |
| 4   | W     | 91/137 (66%)      | 88 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 4   | WA    | 79/137 (58%)      | 74 (94%)    | 5 (6%)    | 0        | 100         | 100 |
| 4   | WC    | 91/137 (66%)      | 88 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 4   | WD    | 79/137 (58%)      | 74 (94%)    | 5 (6%)    | 0        | 100         | 100 |
| 4   | WF    | 91/137 (66%)      | 88 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 4   | WG    | 79/137 (58%)      | 74 (94%)    | 5 (6%)    | 0        | 100         | 100 |
| 4   | X     | 81/137 (59%)      | 73 (90%)    | 8 (10%)   | 0        | 100         | 100 |
| 4   | XC    | 81/137 (59%)      | 73 (90%)    | 8 (10%)   | 0        | 100         | 100 |
| 4   | XF    | 81/137 (59%)      | 73 (90%)    | 8 (10%)   | 0        | 100         | 100 |
| 4   | Y     | 79/137 (58%)      | 74 (94%)    | 5 (6%)    | 0        | 100         | 100 |
| 4   | YB    | 91/137 (66%)      | 88 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 4   | YC    | 79/137 (58%)      | 74 (94%)    | 5 (6%)    | 0        | 100         | 100 |
| 4   | YE    | 91/137 (66%)      | 88 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 4   | YF    | 79/137 (58%)      | 74 (94%)    | 5 (6%)    | 0        | 100         | 100 |
| 4   | ZB    | 81/137 (59%)      | 73 (90%)    | 8 (10%)   | 0        | 100         | 100 |
| 4   | ZE    | 81/137 (59%)      | 73 (90%)    | 8 (10%)   | 0        | 100         | 100 |
| All | All   | 30464/55624 (55%) | 28968 (95%) | 1462 (5%) | 34 (0%)  | 49          | 83  |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 243 | ASP  |
| 2   | B     | 243 | ASP  |
| 2   | J     | 243 | ASP  |
| 2   | T     | 243 | ASP  |
| 2   | AA    | 243 | ASP  |
| 2   | GA    | 243 | ASP  |
| 2   | MA    | 243 | ASP  |
| 2   | SA    | 243 | ASP  |
| 2   | YA    | 243 | ASP  |
| 2   | EB    | 243 | ASP  |
| 2   | KB    | 243 | ASP  |
| 2   | QB    | 243 | ASP  |
| 2   | WB    | 243 | ASP  |
| 2   | CC    | 243 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | IC    | 243 | ASP  |
| 2   | OC    | 243 | ASP  |
| 2   | UC    | 243 | ASP  |
| 2   | AD    | 243 | ASP  |
| 2   | GD    | 243 | ASP  |
| 2   | MD    | 243 | ASP  |
| 2   | SD    | 243 | ASP  |
| 2   | YD    | 243 | ASP  |
| 2   | EE    | 243 | ASP  |
| 2   | KE    | 243 | ASP  |
| 2   | QE    | 243 | ASP  |
| 2   | WE    | 243 | ASP  |
| 2   | CF    | 243 | ASP  |
| 2   | IF    | 243 | ASP  |
| 2   | OF    | 243 | ASP  |
| 2   | UF    | 243 | ASP  |
| 2   | AG    | 243 | ASP  |
| 2   | GG    | 243 | ASP  |
| 2   | MG    | 243 | ASP  |
| 2   | SG    | 243 | ASP  |

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

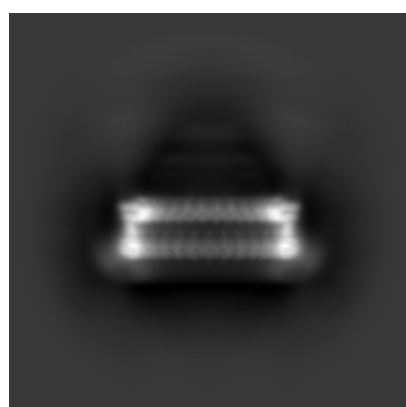
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43328. These allow visual inspection of the internal detail of the map and identification of artifacts.

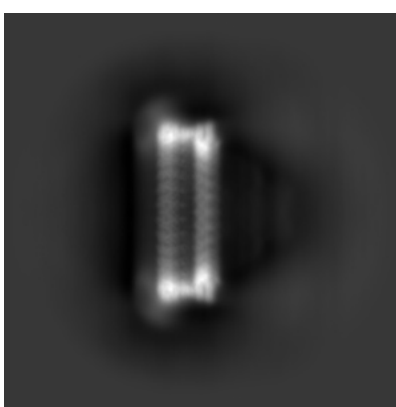
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

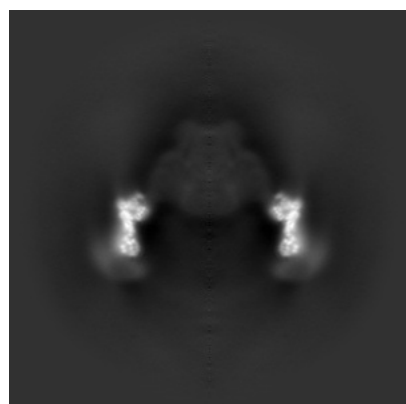


Z

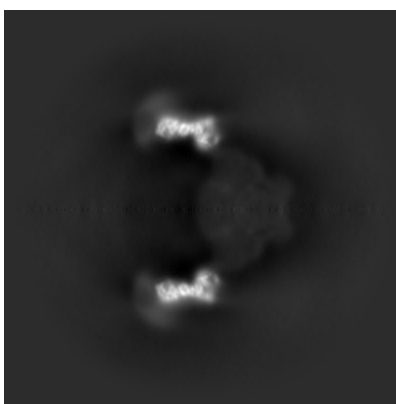
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

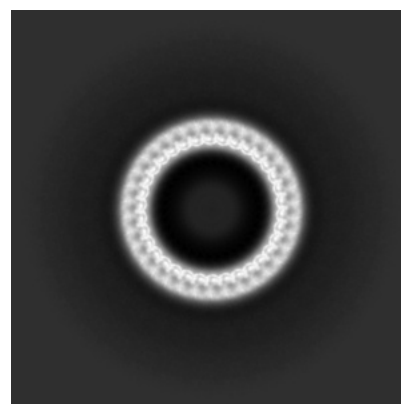
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

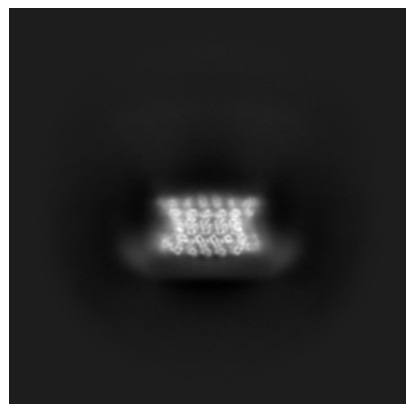


Z Index: 256

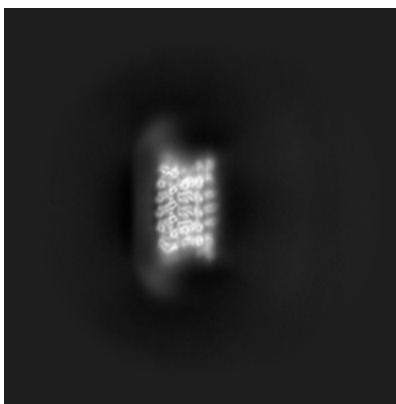
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

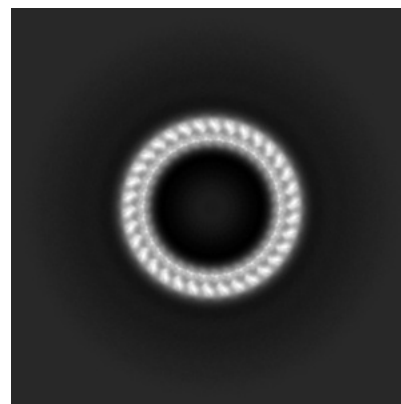
### 6.3.1 Primary map



X Index: 157



Y Index: 157

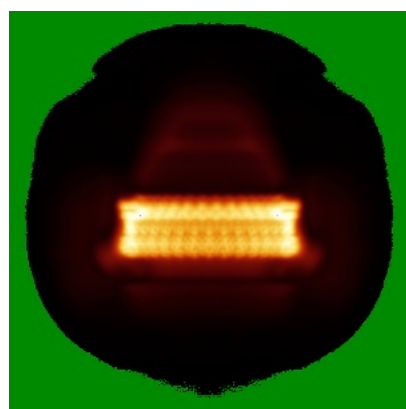


Z Index: 252

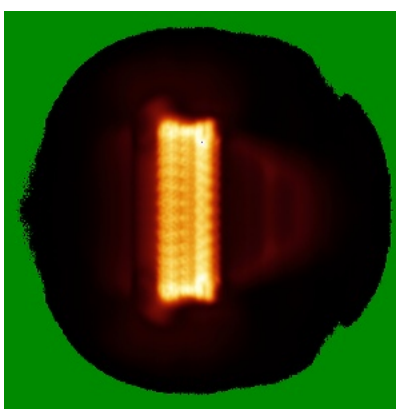
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

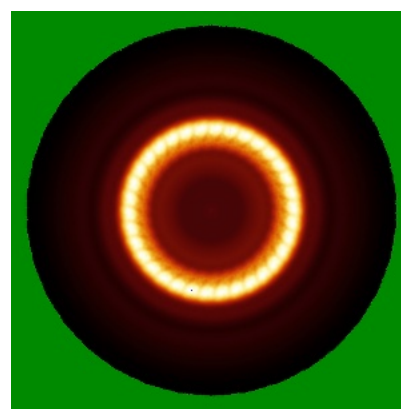
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

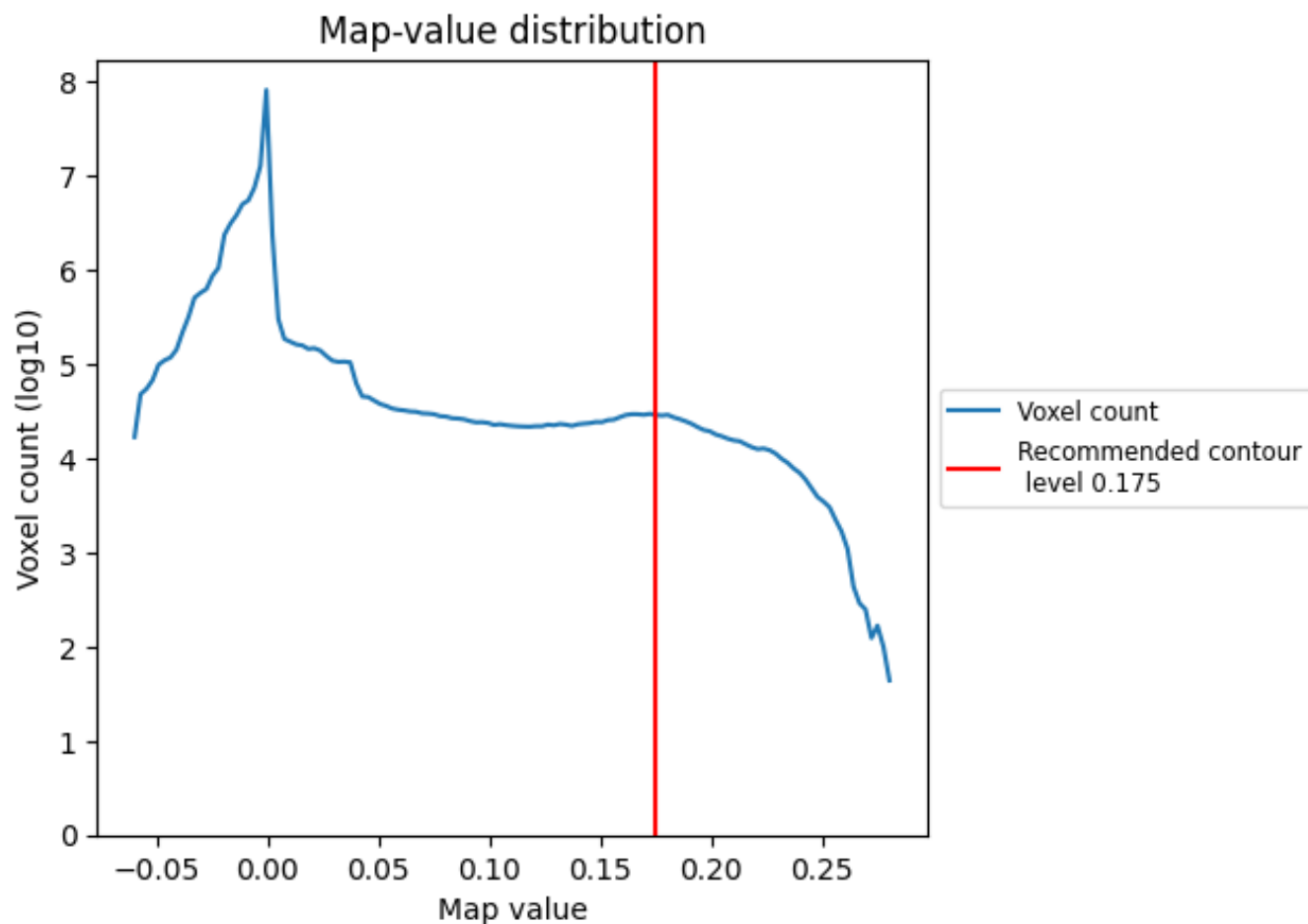
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

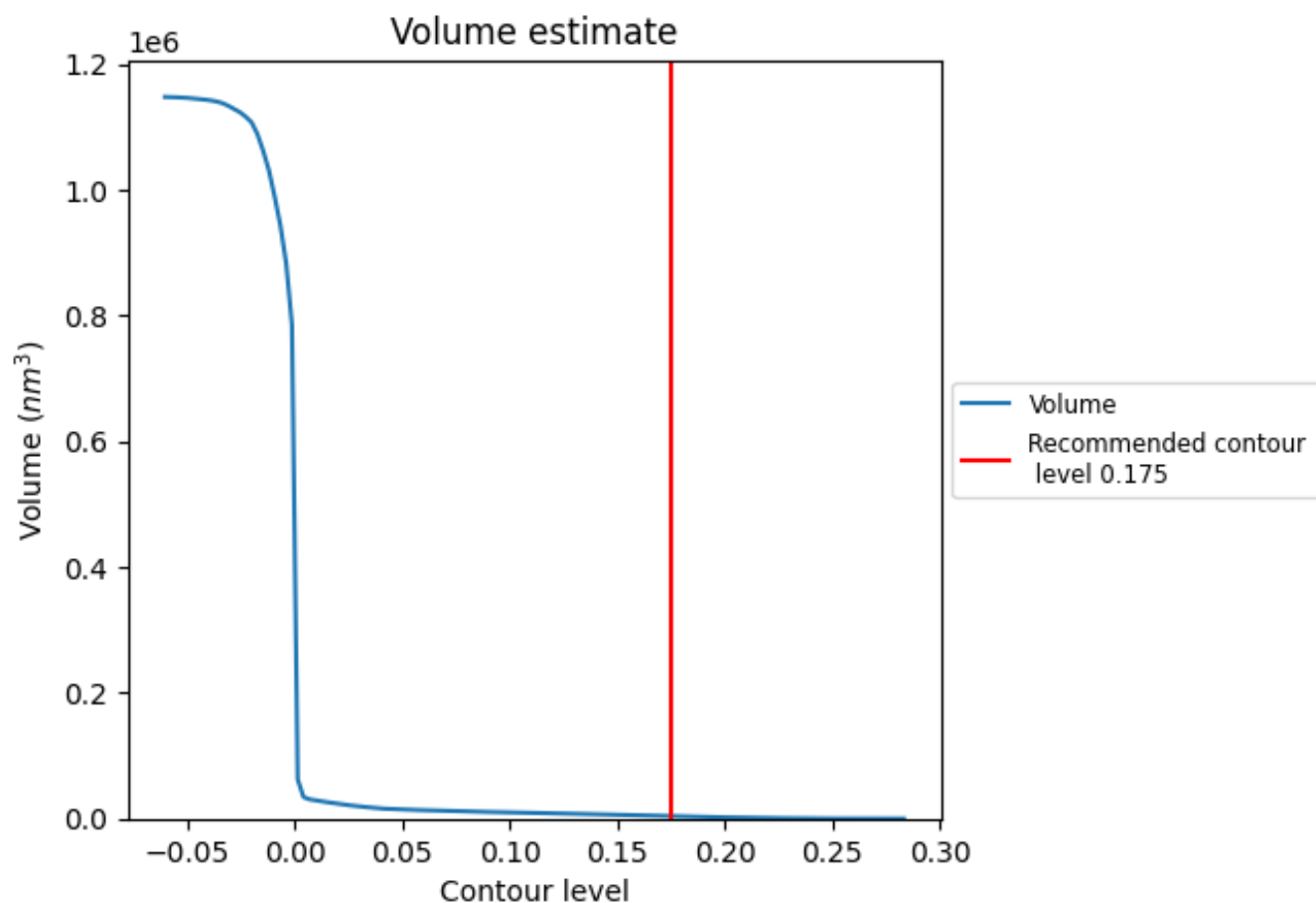
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

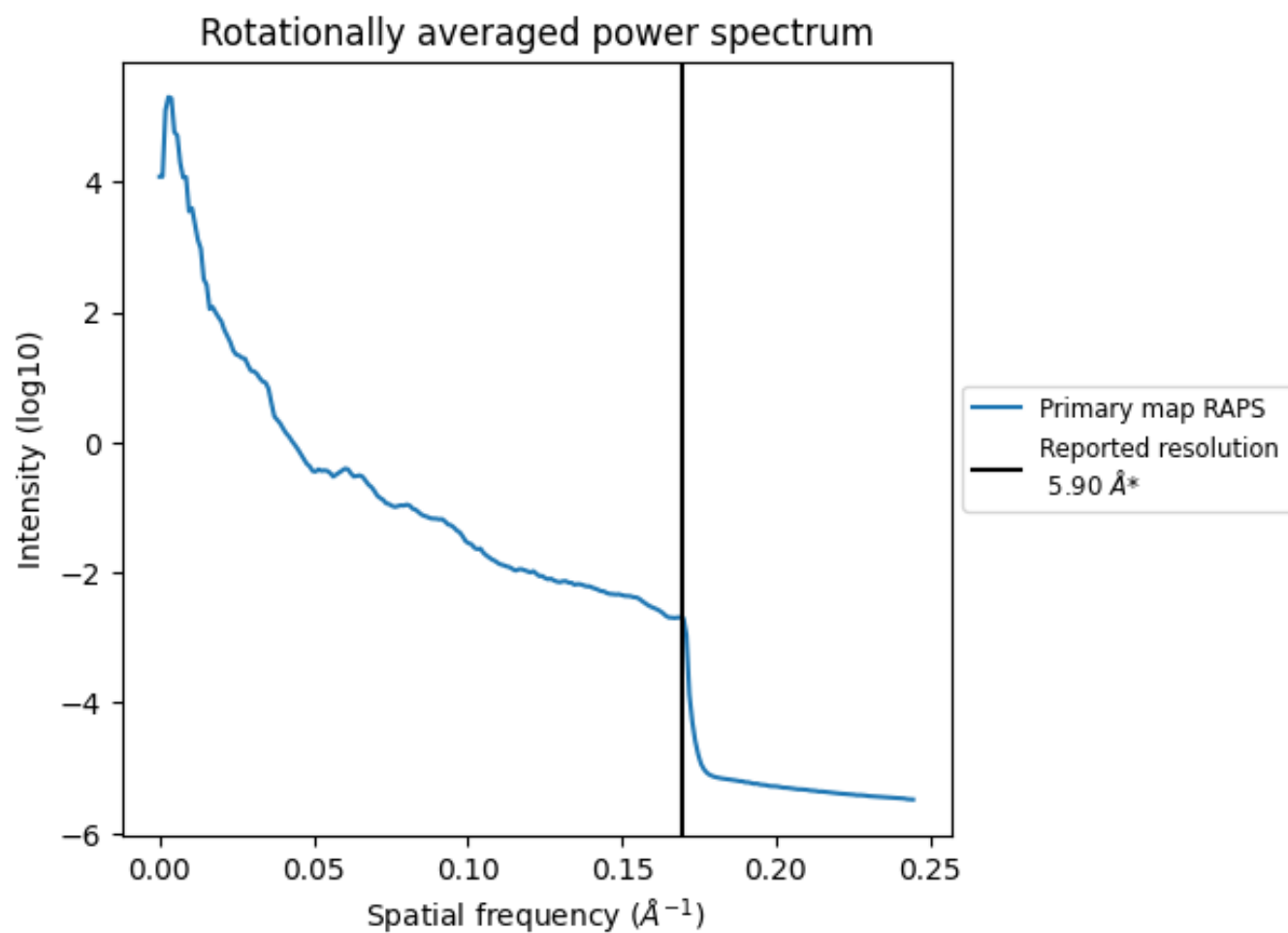
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $4028 \text{ nm}^3$ ; this corresponds to an approximate mass of 3639 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.169 Å<sup>-1</sup>

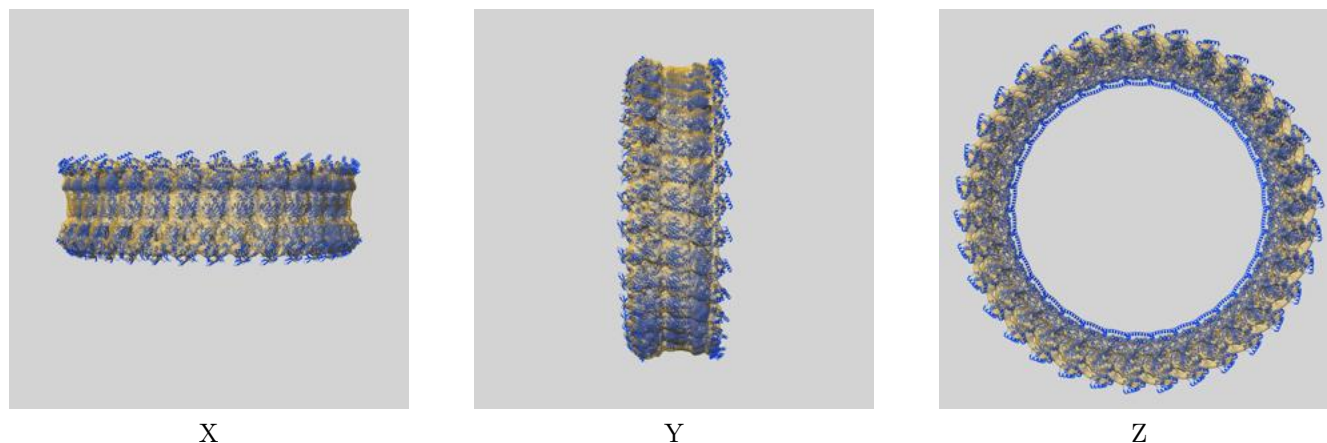
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

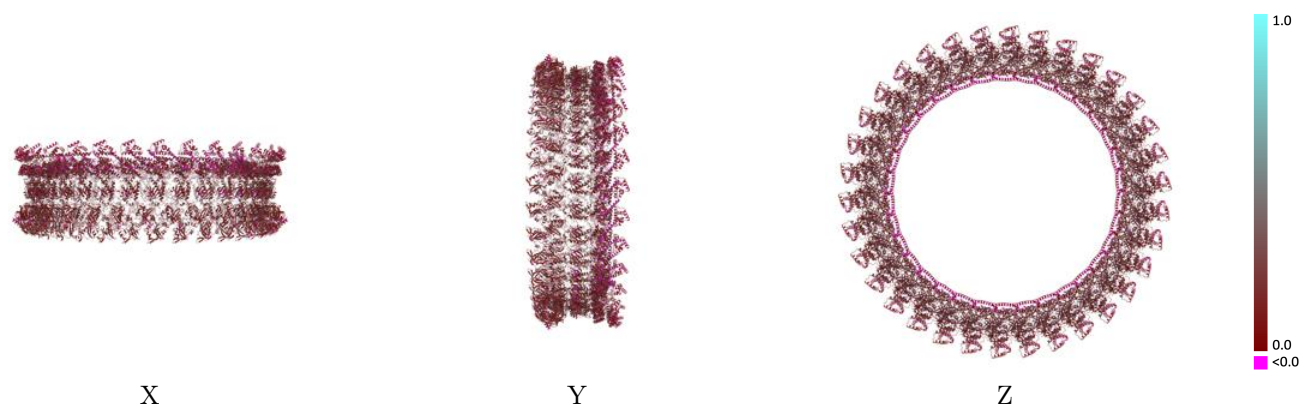
This section contains information regarding the fit between EMDB map EMD-43328 and PDB model 8VKR. Per-residue inclusion information can be found in section [3](#) on page [22](#).

### 9.1 Map-model overlay [i](#)



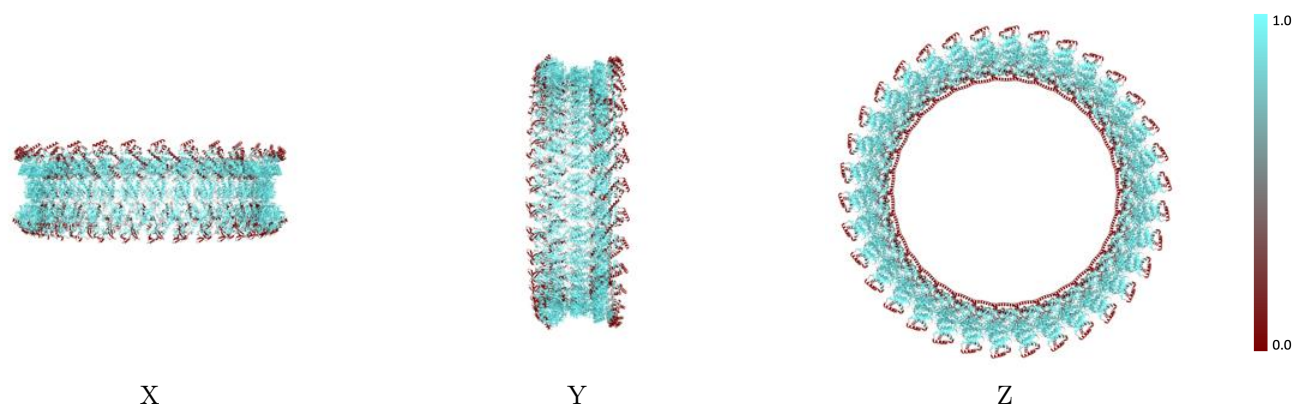
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



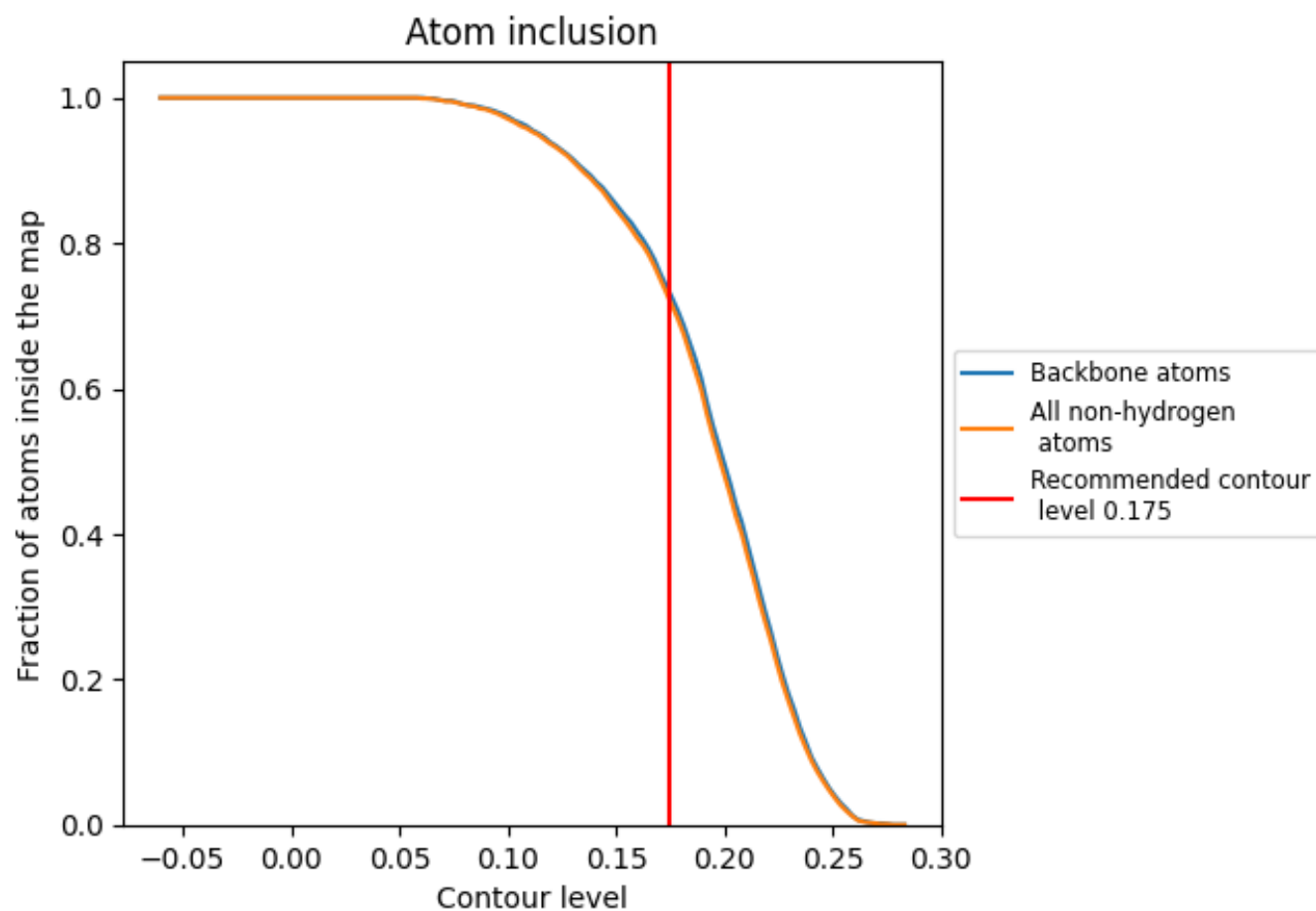
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.175).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.175) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7200   |  0.1760   |
| A     |  0.2270   |  0.0810   |
| AA    |  0.7330   |  0.1670   |
| AB    |  0.4850   |  0.1760   |
| AC    |  0.9470   |  0.2060   |
| AD    |  0.7320   |  0.1650   |
| AE    |  0.4820   |  0.1750   |
| AF    |  0.9520   |  0.2090   |
| AG    |  0.7320   |  0.1680   |
| B     |  0.7330   |  0.1680   |
| BA    |  0.7280   |  0.1930   |
| BB    |  0.9660   |  0.1860   |
| BC    |  0.2270   |  0.0900   |
| BD    |  0.7270   |  0.1930   |
| BE    |  0.9660  |  0.1860  |
| BF    |  0.2270 |  0.0780 |
| BG    |  0.7280 |  0.1900 |
| C     |  0.7270 |  0.1920 |
| CA    |  0.4820 |  0.1730 |
| CB    |  0.9500 |  0.2020 |
| CC    |  0.7320 |  0.1650 |
| CD    |  0.4870 |  0.1790 |
| CE    |  0.9500 |  0.2090 |
| CF    |  0.7310 |  0.1680 |
| CG    |  0.4850 |  0.1770 |
| D     |  0.4820 |  0.1740 |
| DA    |  0.9660 |  0.1880 |
| DB    |  0.2270 |  0.0840 |
| DC    |  0.7280 |  0.1910 |
| DD    |  0.9660 |  0.1810 |
| DE    |  0.2270 |  0.0880 |
| DF    |  0.7250 |  0.1920 |
| DG    |  0.9660 |  0.1890 |
| E     |  0.9660 |  0.1900 |
| EA    |  0.9500 |  0.2040 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| EB    |  0.7310   |  0.1640   |
| EC    |  0.4850   |  0.1740   |
| ED    |  0.9500   |  0.2100   |
| EE    |  0.7330   |  0.1650   |
| EF    |  0.4820   |  0.1830   |
| EG    |  0.9470   |  0.2030   |
| F     |  0.2270   |  0.0820   |
| FA    |  0.2270   |  0.0820   |
| FB    |  0.7250   |  0.1940   |
| FC    |  0.9660   |  0.1850   |
| FD    |  0.2270   |  0.0930   |
| FE    |  0.7260   |  0.1900   |
| FF    |  0.9630   |  0.1860   |
| FG    |  0.2270   |  0.0770   |
| G     |  0.7330   |  0.1690   |
| GA    |  0.7330   |  0.1660   |
| GB    |  0.4820   |  0.1790   |
| GC    |  0.9500   |  0.1990   |
| GD    |  0.7320   |  0.1640   |
| GE    |  0.4850  |  0.1810  |
| GF    |  0.9450 |  0.2060 |
| GG    |  0.7320 |  0.1670 |
| H     |  0.9470 |  0.2040 |
| HA    |  0.7260 |  0.1930 |
| HB    |  0.9660 |  0.1850 |
| HC    |  0.2270 |  0.0920 |
| HD    |  0.7260 |  0.1910 |
| HE    |  0.9660 |  0.1850 |
| HF    |  0.2270 |  0.0760 |
| HG    |  0.7300 |  0.1930 |
| I     |  0.2270 |  0.0790 |
| IA    |  0.4820 |  0.1800 |
| IB    |  0.9500 |  0.1970 |
| IC    |  0.7330 |  0.1640 |
| ID    |  0.4850 |  0.1770 |
| IE    |  0.9470 |  0.2090 |
| IF    |  0.7330 |  0.1680 |
| IG    |  0.4850 |  0.1780 |
| J     |  0.7330 |  0.1670 |
| JA    |  0.9660 |  0.1890 |
| JB    |  0.2270 |  0.0830 |
| JC    |  0.7300 |  0.1950 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| JD    |  0.9630   |  0.1860   |
| JE    |  0.2270   |  0.0880   |
| JF    |  0.7300   |  0.1910   |
| JG    |  0.9630   |  0.1850   |
| K     |  0.7260   |  0.1920   |
| KA    |  0.9500   |  0.2050   |
| KB    |  0.7330   |  0.1630   |
| KC    |  0.4870   |  0.1750   |
| KD    |  0.9550   |  0.2060   |
| KE    |  0.7320   |  0.1650   |
| KF    |  0.4850   |  0.1780   |
| KG    |  0.9520   |  0.2100   |
| L     |  0.4870   |  0.1820   |
| LA    |  0.2220   |  0.0850   |
| LB    |  0.7280   |  0.1940   |
| LC    |  0.9660   |  0.1810   |
| LD    |  0.2270   |  0.0870   |
| LE    |  0.7260   |  0.1910   |
| LF    |  0.9660  |  0.1870  |
| LG    |  0.2270 |  0.0760 |
| M     |  0.7280 |  0.1930 |
| MA    |  0.7330 |  0.1650 |
| MB    |  0.4850 |  0.1730 |
| MC    |  0.9470 |  0.2080 |
| MD    |  0.7330 |  0.1650 |
| ME    |  0.4820 |  0.1830 |
| MF    |  0.9470 |  0.2100 |
| MG    |  0.7330 |  0.1680 |
| N     |  0.4870 |  0.1790 |
| NA    |  0.7250 |  0.1940 |
| NB    |  0.9660 |  0.1840 |
| NC    |  0.2270 |  0.0870 |
| ND    |  0.7260 |  0.1920 |
| NE    |  0.9660 |  0.1880 |
| NF    |  0.2270 |  0.0790 |
| NG    |  0.7280 |  0.1900 |
| O     |  0.9660 |  0.1930 |
| OA    |  0.4850 |  0.1770 |
| OB    |  0.9520 |  0.2000 |
| OC    |  0.7330 |  0.1640 |
| OD    |  0.4870 |  0.1820 |
| OE    |  0.9470 |  0.2080 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| OF    |  0.7330   |  0.1670   |
| OG    |  0.4890   |  0.1800   |
| P     |  0.9660   |  0.1860   |
| PA    |  0.9630   |  0.1900   |
| PB    |  0.2270   |  0.0900   |
| PC    |  0.7280   |  0.1940   |
| PD    |  0.9630   |  0.1870   |
| PE    |  0.2270   |  0.0860   |
| PF    |  0.7270   |  0.1890   |
| PG    |  0.9660   |  0.1890   |
| Q     |  0.9500   |  0.2070   |
| QA    |  0.9520   |  0.2020   |
| QB    |  0.7320   |  0.1620   |
| QC    |  0.4850   |  0.1820   |
| QD    |  0.9520   |  0.2090   |
| QE    |  0.7310   |  0.1660   |
| QF    |  0.4850   |  0.1790   |
| QG    |  0.9500   |  0.2050   |
| R     |  0.9470  |  0.2030  |
| RA    |  0.2270 |  0.0830 |
| RB    |  0.7280 |  0.1900 |
| RC    |  0.9660 |  0.1840 |
| RD    |  0.2270 |  0.0850 |
| RE    |  0.7250 |  0.1900 |
| RF    |  0.9660 |  0.1890 |
| RG    |  0.2270 |  0.0760 |
| S     |  0.2270 |  0.0770 |
| SA    |  0.7320 |  0.1650 |
| SB    |  0.4870 |  0.1760 |
| SC    |  0.9500 |  0.2080 |
| SD    |  0.7330 |  0.1650 |
| SE    |  0.4870 |  0.1810 |
| SF    |  0.9470 |  0.2060 |
| SG    |  0.7320 |  0.1680 |
| T     |  0.7330 |  0.1670 |
| TA    |  0.7290 |  0.1920 |
| TB    |  0.9630 |  0.1850 |
| TC    |  0.2270 |  0.0880 |
| TD    |  0.7260 |  0.1900 |
| TE    |  0.9630 |  0.1860 |
| TF    |  0.2270 |  0.0810 |
| TG    |  0.7260 |  0.1910 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| UA    |  0.4850   |  0.1760   |
| UB    |  0.9470   |  0.2020   |
| UC    |  0.7310   |  0.1630   |
| UD    |  0.4870   |  0.1790   |
| UE    |  0.9520   |  0.2100   |
| UF    |  0.7330   |  0.1680   |
| UG    |  0.4850   |  0.1780   |
| V     |  0.7260   |  0.1910   |
| VA    |  0.9630   |  0.1870   |
| VB    |  0.2270   |  0.0900   |
| VC    |  0.7250   |  0.1930   |
| VD    |  0.9630   |  0.1820   |
| VE    |  0.2270   |  0.0810   |
| VF    |  0.7280   |  0.1930   |
| VG    |  0.9660   |  0.1870   |
| W     |  0.4850   |  0.1780   |
| WA    |  0.9470   |  0.2030   |
| WB    |  0.7330   |  0.1650   |
| WC    |  0.4870  |  0.1820  |
| WD    |  0.9470 |  0.2060 |
| WE    |  0.7330 |  0.1660 |
| WF    |  0.4850 |  0.1770 |
| WG    |  0.9470 |  0.2070 |
| X     |  0.9660 |  0.1890 |
| XA    |  0.2270 |  0.0840 |
| XB    |  0.7300 |  0.1940 |
| XC    |  0.9660 |  0.1850 |
| XD    |  0.2270 |  0.0860 |
| XE    |  0.7250 |  0.1910 |
| XF    |  0.9630 |  0.1890 |
| Y     |  0.9470 |  0.2000 |
| YA    |  0.7330 |  0.1630 |
| YB    |  0.4850 |  0.1750 |
| YC    |  0.9520 |  0.2120 |
| YD    |  0.7330 |  0.1650 |
| YE    |  0.4850 |  0.1770 |
| YF    |  0.9520 |  0.2100 |
| Z     |  0.2270 |  0.0800 |
| ZA    |  0.7280 |  0.1930 |
| ZB    |  0.9660 |  0.1830 |
| ZC    |  0.2270 |  0.0890 |
| ZD    |  0.7280 |  0.1920 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| ZE    |  0.9630 |  0.1880 |
| ZF    |  0.2270 |  0.0790 |