



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:22 PM UTC

PDB ID : 3A0H / pdb\_00003a0h  
Title : Crystal structure of I-substituted Photosystem II complex  
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.  
Deposited on : 2009-03-17  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

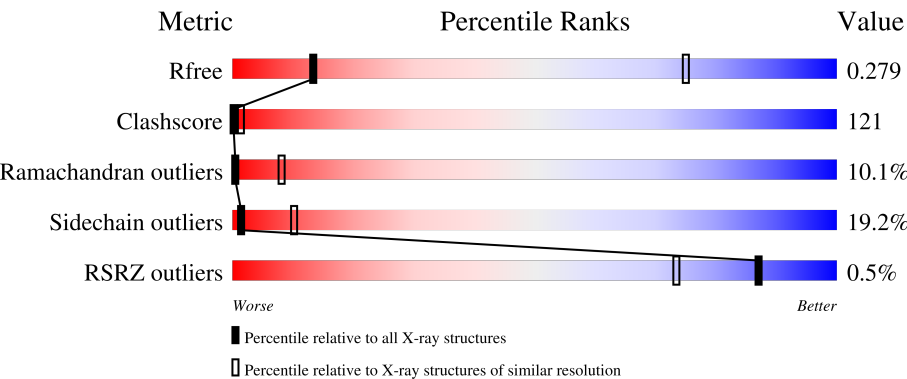
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 Å.

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



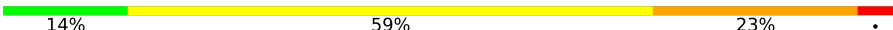
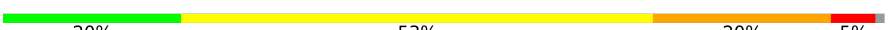
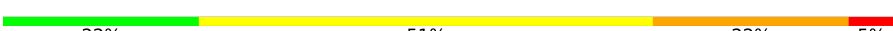
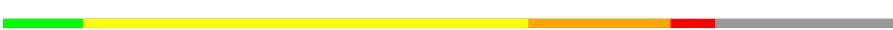
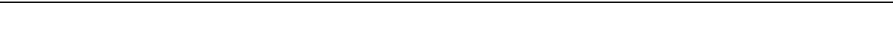
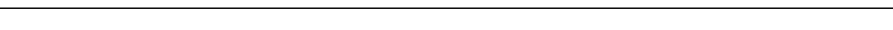
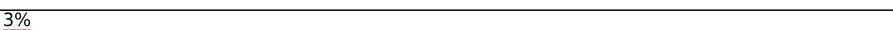
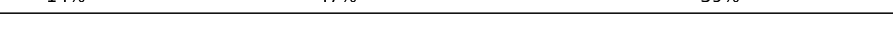
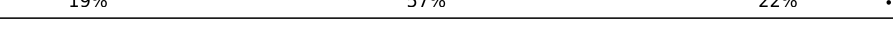
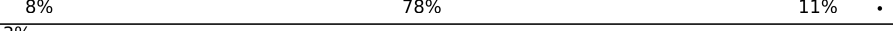
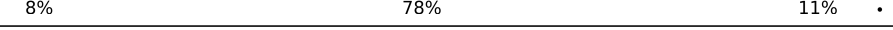
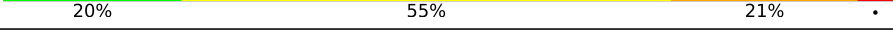
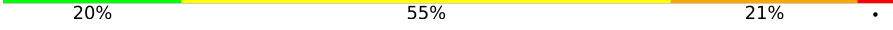
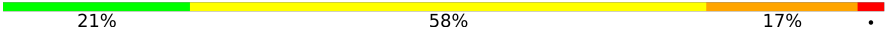
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1082 (4.20-3.80)                                      |
| Clashscore            | 190562                      | 1129 (4.20-3.80)                                      |
| Ramachandran outliers | 187476                      | 1064 (4.20-3.80)                                      |
| Sidechain outliers    | 187428                      | 1055 (4.20-3.80)                                      |
| RSRZ outliers         | 180081                      | 1082 (4.20-3.80)                                      |

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

| Mol | Chain | Length | Quality of chain                                |
|-----|-------|--------|-------------------------------------------------|
| 1   | A     | 344    | <div><div>%</div><div>11%56%26% . .</div></div> |
| 1   | a     | 344    | <div><div>%</div><div>11%56%26% . .</div></div> |
| 2   | B     | 488    | <div><div>%</div><div>17%56%24% .</div></div>   |
| 2   | b     | 488    | <div><div>%</div><div>17%56%24% .</div></div>   |
| 3   | C     | 447    | <div><div>%</div><div>14%59%23% .</div></div>   |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | c     | 447    |    |
| 4   | D     | 340    |    |
| 4   | d     | 340    |    |
| 5   | E     | 83     |    |
| 5   | e     | 83     |    |
| 6   | F     | 44     |    |
| 6   | f     | 44     |    |
| 7   | H     | 64     |    |
| 7   | h     | 64     |    |
| 8   | I     | 35     |    |
| 8   | i     | 35     |    |
| 9   | J     | 40     |    |
| 9   | j     | 40     |  |
| 10  | K     | 36     |  |
| 10  | k     | 36     |  |
| 11  | L     | 37     |  |
| 11  | l     | 37     |  |
| 12  | M     | 36     |  |
| 12  | m     | 36     |  |
| 13  | O     | 242    |  |
| 13  | o     | 242    |  |
| 14  | T     | 30     |  |
| 14  | t     | 30     |  |
| 15  | U     | 98     |  |
| 15  | u     | 98     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16  | V     | 137    |                  |
| 16  | v     | 137    |                  |
| 17  | X     | 34     |                  |
| 17  | x     | 34     |                  |
| 18  | Y     | 28     |                  |
| 18  | y     | 28     |                  |
| 19  | N     | 23     |                  |
| 19  | n     | 23     |                  |
| 20  | Z     | 62     |                  |
| 20  | z     | 62     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | CLA  | A     | 1003 | X         | -        | X       | -                |
| 22  | CLA  | A     | 1006 | X         | -        | X       | -                |
| 22  | CLA  | A     | 1007 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1009 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1010 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1011 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1012 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1013 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1014 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1015 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1016 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1018 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1019 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1020 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1021 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1022 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1023 | X         | -        | X       | -                |
| 22  | CLA  | B     | 1024 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1025 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1026 | X         | -        | X       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | CLA  | C     | 1027 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1028 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1029 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1030 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1031 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1032 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1033 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1035 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1036 | X         | -        | X       | -                |
| 22  | CLA  | C     | 1037 | X         | -        | X       | -                |
| 22  | CLA  | D     | 1004 | X         | -        | X       | -                |
| 22  | CLA  | D     | 1005 | X         | -        | X       | -                |
| 22  | CLA  | D     | 1008 | X         | -        | X       | -                |
| 22  | CLA  | H     | 1017 | X         | -        | X       | -                |
| 22  | CLA  | K     | 1034 | X         | -        | X       | -                |
| 22  | CLA  | a     | 6003 | X         | -        | X       | -                |
| 22  | CLA  | a     | 6006 | X         | -        | X       | -                |
| 22  | CLA  | a     | 6007 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6009 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6010 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6011 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6012 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6013 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6014 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6015 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6016 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6018 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6019 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6020 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6021 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6022 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6023 | X         | -        | X       | -                |
| 22  | CLA  | b     | 6024 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6025 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6026 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6027 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6028 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6029 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6030 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6031 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6032 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6033 | X         | -        | X       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | CLA  | c     | 6035 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6036 | X         | -        | X       | -                |
| 22  | CLA  | c     | 6037 | X         | -        | X       | -                |
| 22  | CLA  | d     | 6004 | X         | -        | X       | -                |
| 22  | CLA  | d     | 6005 | X         | -        | X       | -                |
| 22  | CLA  | d     | 6008 | X         | -        | X       | -                |
| 22  | CLA  | h     | 6017 | X         | -        | X       | -                |
| 22  | CLA  | k     | 6034 | X         | -        | X       | -                |
| 23  | PHO  | A     | 1038 | X         | -        | X       | -                |
| 23  | PHO  | D     | 1039 | X         | -        | X       | -                |
| 23  | PHO  | a     | 6038 | X         | -        | X       | -                |
| 23  | PHO  | d     | 6039 | X         | -        | X       | -                |
| 24  | PQ9  | A     | 1043 | -         | -        | X       | -                |
| 24  | PQ9  | D     | 1042 | -         | -        | X       | -                |
| 24  | PQ9  | a     | 6043 | -         | -        | X       | -                |
| 24  | PQ9  | d     | 6042 | -         | -        | X       | -                |
| 25  | BCR  | A     | 1044 | -         | -        | X       | -                |
| 25  | BCR  | B     | 1045 | -         | -        | X       | -                |
| 25  | BCR  | B     | 1047 | -         | -        | X       | -                |
| 25  | BCR  | B     | 1048 | -         | -        | X       | -                |
| 25  | BCR  | C     | 1052 | -         | -        | X       | -                |
| 25  | BCR  | C     | 1054 | -         | -        | X       | -                |
| 25  | BCR  | D     | 1050 | -         | -        | X       | -                |
| 25  | BCR  | H     | 1049 | -         | -        | X       | -                |
| 25  | BCR  | K     | 1051 | -         | -        | X       | -                |
| 25  | BCR  | T     | 6046 | -         | -        | X       | -                |
| 25  | BCR  | T     | 6048 | -         | -        | X       | -                |
| 25  | BCR  | a     | 6044 | -         | -        | X       | -                |
| 25  | BCR  | b     | 6045 | -         | -        | X       | -                |
| 25  | BCR  | b     | 6047 | -         | -        | X       | -                |
| 25  | BCR  | c     | 6054 | -         | -        | X       | -                |
| 25  | BCR  | d     | 6050 | -         | -        | X       | -                |
| 25  | BCR  | h     | 6049 | -         | -        | X       | -                |
| 25  | BCR  | k     | 6051 | -         | -        | X       | -                |
| 25  | BCR  | k     | 6052 | -         | -        | X       | -                |
| 25  | BCR  | t     | 1046 | -         | -        | X       | -                |
| 26  | LHG  | A     | 1063 | -         | -        | X       | -                |
| 26  | LHG  | a     | 6063 | -         | -        | X       | -                |
| 27  | IOD  | B     | 1067 | -         | -        | X       | X                |
| 27  | IOD  | D     | 1064 | -         | -        | X       | -                |
| 27  | IOD  | D     | 1068 | -         | -        | X       | X                |
| 27  | IOD  | T     | 1066 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 27  | IOD  | b     | 6067 | -         | -        | -       | X                |
| 27  | IOD  | d     | 6064 | -         | -        | X       | -                |
| 27  | IOD  | d     | 6068 | -         | -        | X       | -                |
| 27  | IOD  | t     | 6066 | -         | -        | X       | -                |
| 28  | MGE  | B     | 1060 | -         | -        | X       | -                |
| 28  | MGE  | D     | 1059 | -         | -        | X       | -                |
| 28  | MGE  | D     | 1062 | -         | -        | X       | -                |
| 28  | MGE  | L     | 1061 | -         | -        | X       | -                |
| 28  | MGE  | b     | 6060 | -         | -        | X       | -                |
| 28  | MGE  | d     | 6059 | -         | -        | X       | -                |
| 28  | MGE  | d     | 6062 | -         | -        | X       | -                |
| 28  | MGE  | l     | 6061 | -         | -        | X       | -                |
| 29  | DGD  | B     | 1058 | -         | -        | X       | -                |
| 29  | DGD  | C     | 1055 | -         | -        | X       | -                |
| 29  | DGD  | C     | 1056 | -         | -        | X       | -                |
| 29  | DGD  | C     | 1057 | -         | -        | X       | -                |
| 29  | DGD  | b     | 6058 | -         | -        | X       | -                |
| 29  | DGD  | c     | 6055 | -         | -        | X       | -                |
| 29  | DGD  | c     | 6056 | -         | -        | X       | -                |
| 29  | DGD  | c     | 6057 | -         | -        | X       | -                |

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 48060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2630  | 1720 | 435 | 460 | 15 |         |         |       |
| 1   | a     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2630  | 1720 | 435 | 460 | 15 |         |         |       |

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3835  | 2518 | 638 | 666 | 13 |         |         |       |
| 2   | b     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3835  | 2518 | 638 | 666 | 13 |         |         |       |

- Molecule 3 is a protein called Photosystem II CP43 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 447      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3455  | 2264 | 576 | 602 | 13 |         |         |       |
| 3   | c     | 447      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3455  | 2264 | 576 | 602 | 13 |         |         |       |

- Molecule 4 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2706  | 1794 | 440 | 460 | 12 |         |         |       |
| 4   | d     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2706  | 1794 | 440 | 460 | 12 |         |         |       |

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 82       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 666   | 434 | 108 | 124 |         |         |       |
| 5   | e     | 82       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 666   | 434 | 108 | 124 |         |         |       |

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 282   | 192 | 46 | 43 | 1 |         |         |       |
| 6   | f     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 282   | 192 | 46 | 43 | 1 |         |         |       |

- Molecule 7 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H     | 64       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 339 | 81 | 85 | 2 |         |         |       |
| 7   | h     | 64       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 339 | 81 | 85 | 2 |         |         |       |

- Molecule 8 is a protein called Photosystem II reaction center protein I.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | I     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 287   | 195 | 45 | 46 | 1 |         |         |       |
| 8   | i     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 287   | 195 | 45 | 46 | 1 |         |         |       |

- Molecule 9 is a protein called Photosystem II reaction center protein J.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | J     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 249   | 170 | 38 | 40 | 1 |         |         |       |
| 9   | j     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 249   | 170 | 38 | 40 | 1 |         |         |       |

- Molecule 10 is a protein called Photosystem II reaction center protein K.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | K     | 36       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 278   | 195 | 38 | 45 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | k     | 36       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 278   | 195 | 38 | 45 |         |         |       |

- Molecule 11 is a protein called Photosystem II reaction center protein L.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | L     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 304   | 202 | 48 | 53 | 1 |         |         |       |
| 11  | l     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 304   | 202 | 48 | 53 | 1 |         |         |       |

- Molecule 12 is a protein called Photosystem II reaction center protein M.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M     | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 283   | 187 | 42 | 53 | 1 |         |         |       |
| 12  | m     | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 283   | 187 | 42 | 53 | 1 |         |         |       |

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | O     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1860  | 1162 | 314 | 380 | 4 |         |         |       |
| 13  | o     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1860  | 1162 | 314 | 380 | 4 |         |         |       |

- Molecule 14 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | T     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 257   | 180 | 36 | 39 | 2 |         |         |       |
| 14  | t     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 257   | 180 | 36 | 39 | 2 |         |         |       |

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15  | U     | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 783   | 496 | 130 | 157 |         |         |       |
| 15  | u     | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 783   | 496 | 130 | 157 |         |         |       |

- Molecule 16 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | V     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 675 | 177 | 208 | 4 |         |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 675 | 177 | 208 | 4 |         |         |       |

- Molecule 17 is a protein called Photosystem II reaction center protein X.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | X     | 34       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 246   | 166 | 36 | 44 |         |         |       |
| 17  | x     | 34       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 246   | 166 | 36 | 44 |         |         |       |

- Molecule 18 is a protein called Photosystem II reaction center protein ycf12.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18  | Y     | 28       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 208   | 137 | 36 | 32 | 3 |         |         |       |
| 18  | y     | 28       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 208   | 137 | 36 | 32 | 3 |         |         |       |

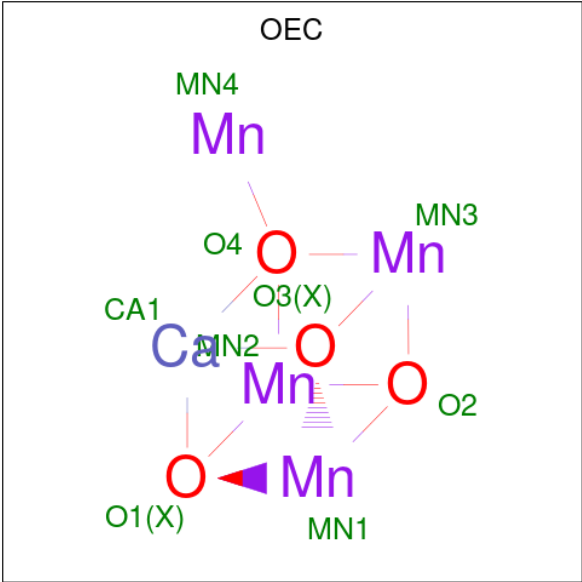
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 19  | N     | 23       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 116   | 69 | 23 | 24 |         |         |       |
| 19  | n     | 23       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 116   | 69 | 23 | 24 |         |         |       |

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

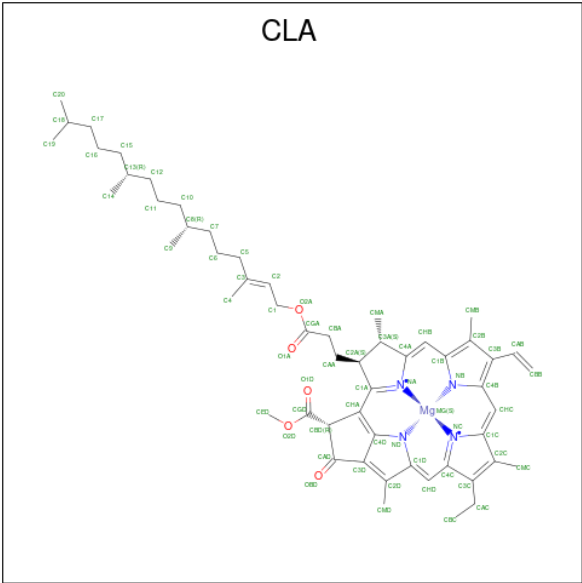
| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |
| 20  | z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |

- Molecule 21 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 21  | A     | 1        | Total | Ca | Mn | 0       | 0       |
|     |       |          | 5     | 1  | 4  |         |         |
| 21  | a     | 1        | Total | Ca | Mn | 0       | 0       |
|     |       |          | 5     | 1  | 4  |         |         |

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | K     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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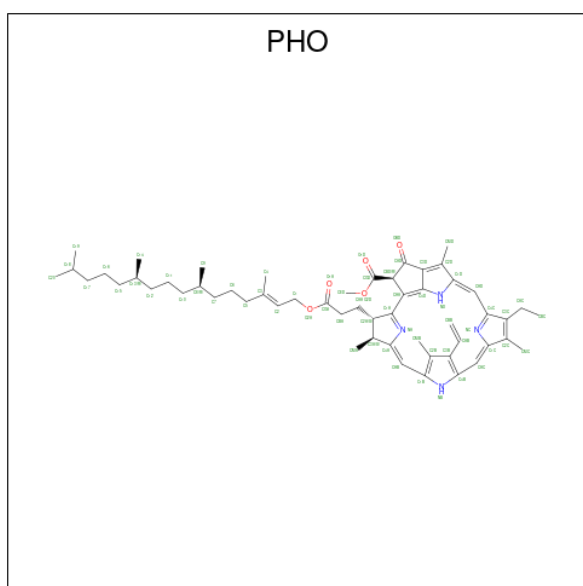
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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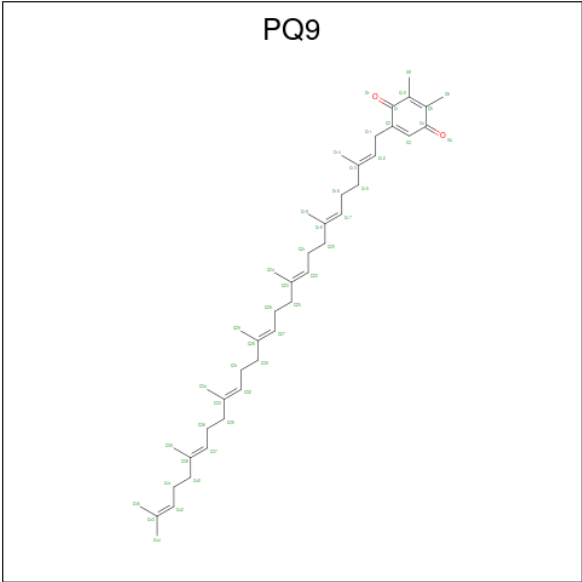
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | h     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | k     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



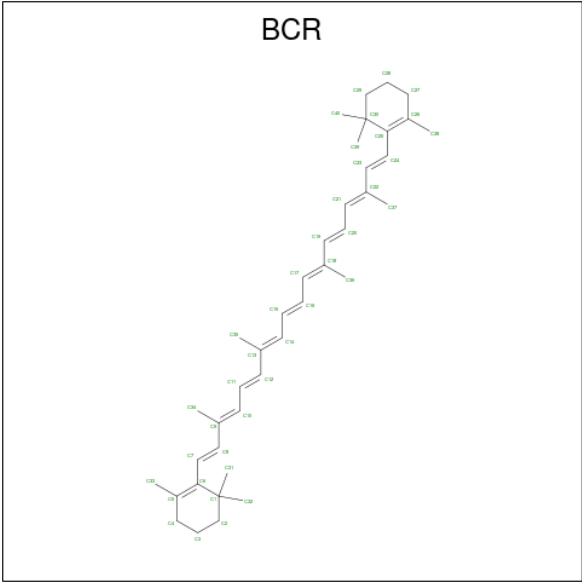
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 23  | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 23  | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 23  | a     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 23  | d     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |

- Molecule 24 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C<sub>43</sub>H<sub>64</sub>O<sub>2</sub>).



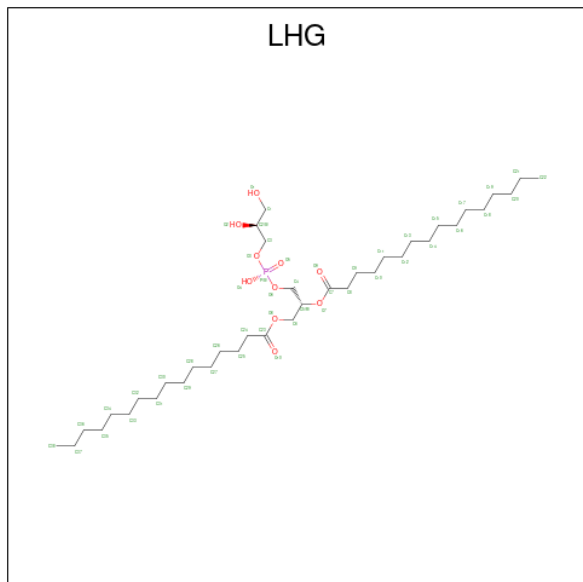
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 24  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |
| 24  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |
| 24  | a     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |
| 24  | d     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | Z     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | h     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | t     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | z     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).

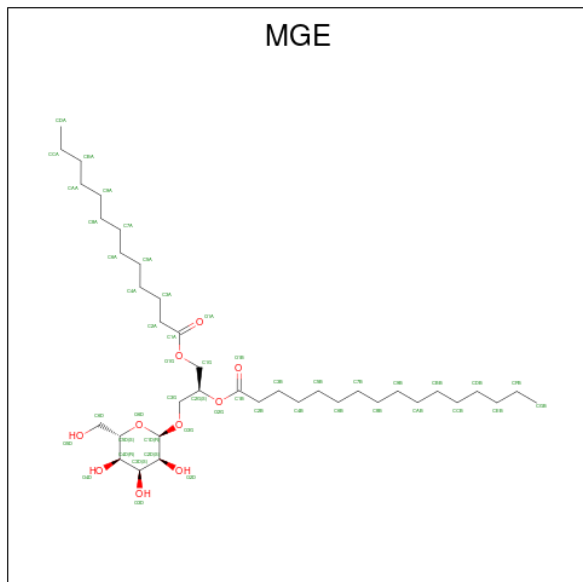


| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 26  | a     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

- Molecule 27 is IODIDE ION (CCD ID: IOD) (formula: I).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 27  | A     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 27  | B     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 27  | D     | 2        | Total | I | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 27  | T     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 27  | a     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 27  | b     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 27  | d     | 2        | Total | I | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 27  | t     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

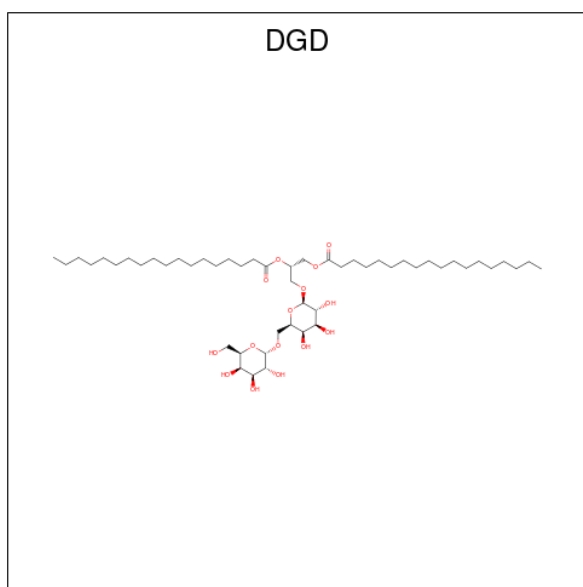
- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula:  $C_{38}H_{72}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 28  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 28  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 28  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 28  | L     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 28  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 28  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 28  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 28  | l     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



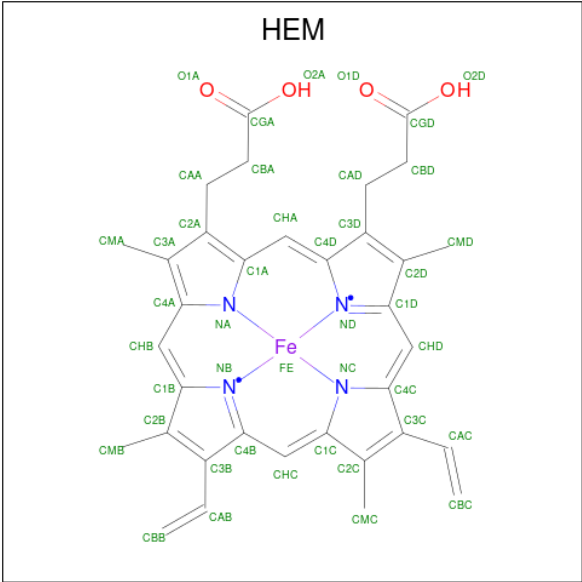


| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 29  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 29  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 29  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 29  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 29  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 29  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 29  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 30  | D     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 30  | a     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).

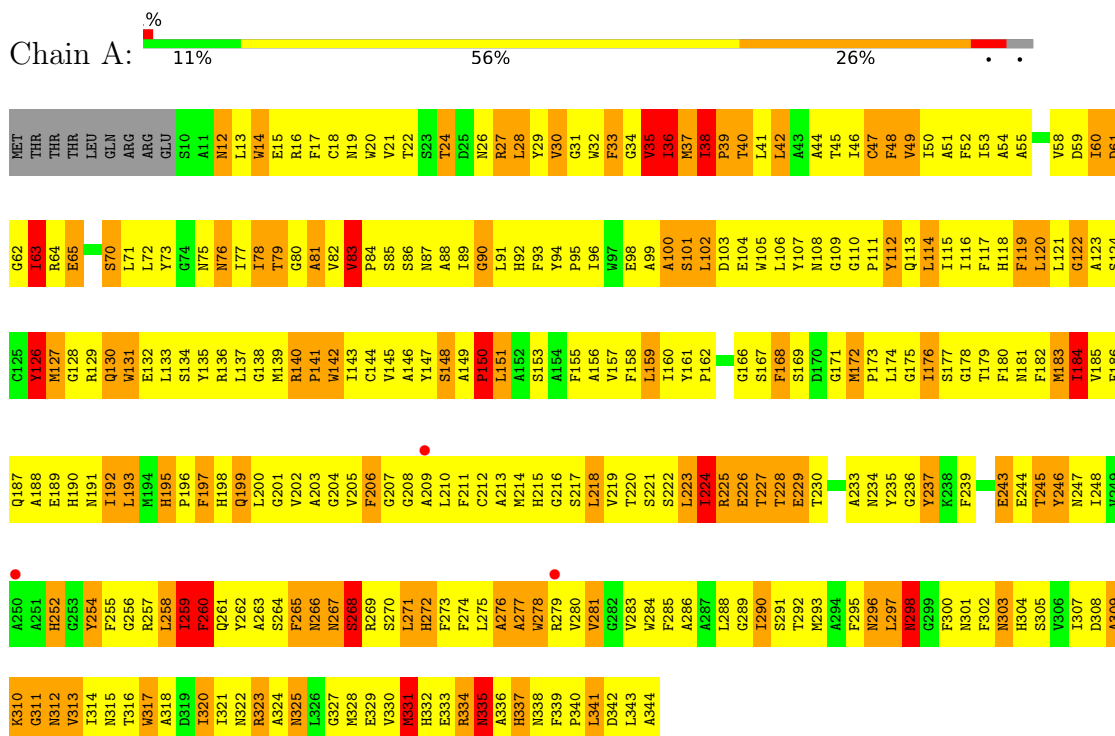


| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 31  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 31  | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 31  | f     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 31  | v     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

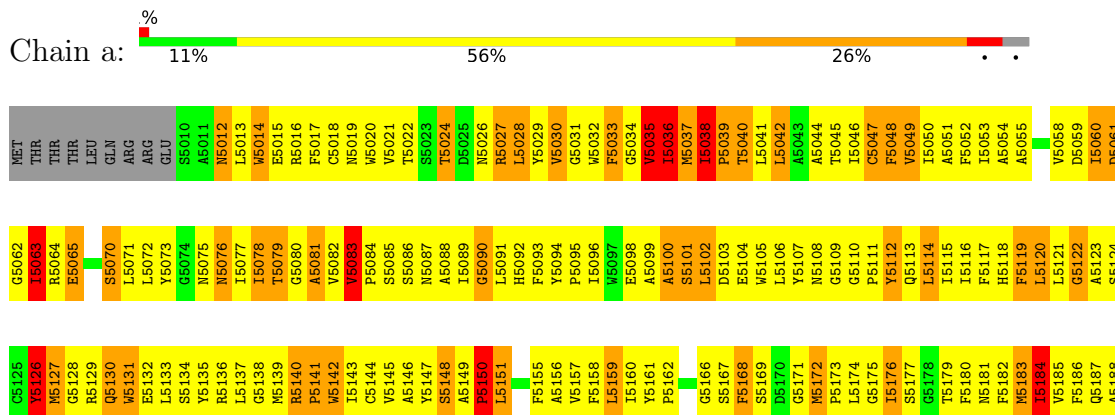
### 3 Residue-property plots

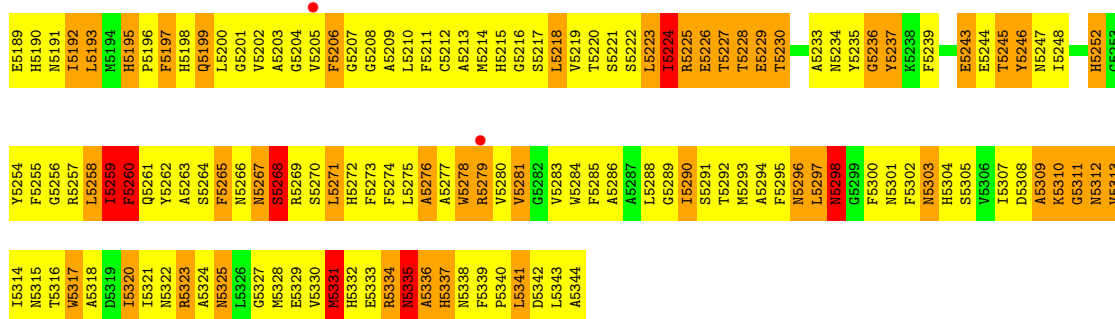
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Photosystem Q(B) protein

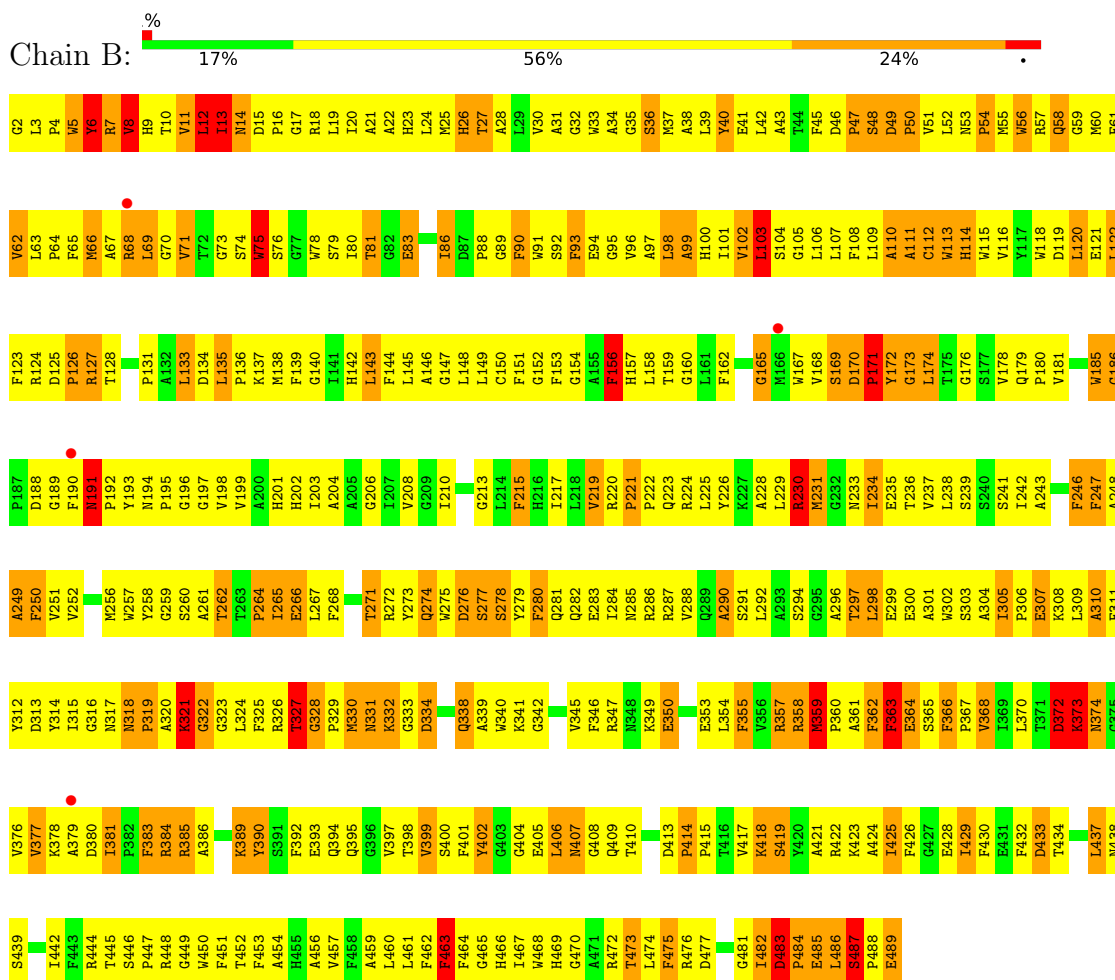


#### • Molecule 1: Photosystem Q(B) protein

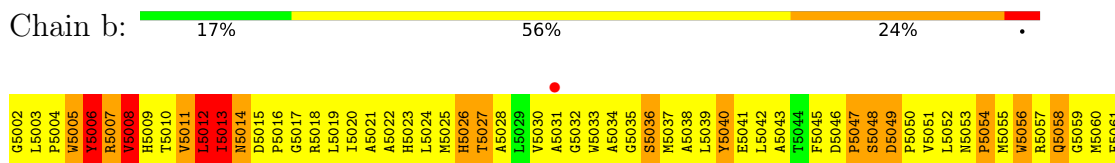




• Molecule 2: Photosystem II core light harvesting protein

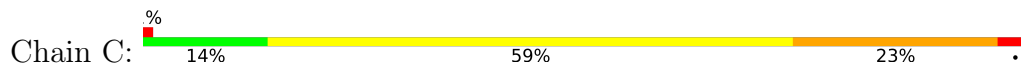


• Molecule 2: Photosystem II core light harvesting protein



|       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|
| V5062 | F5123 | P5187 | F5250 | Y5312 | V5376 | S5439 |
| L5063 | R5124 | D5188 | V5251 | D5313 | V5377 |       |
| P5064 | D5125 | G5189 | F5252 | Y5314 | F5378 | I5442 |
| F5065 | F5190 | F5190 | M5256 | I5315 | A5379 | F5443 |
| A5066 | M5257 | N5191 | M5256 | G5316 | D5380 | R5444 |
| M5067 | R5127 | F5192 | M5257 | N5317 | I5381 | T5445 |
| R5068 | F5128 | Y5193 | Y5258 | N5318 | P5382 | S5446 |
| L5069 | P5131 | N5194 | G5259 | P5319 | F5383 | P5447 |
| G5070 | A5132 | P5195 | S5260 | A5320 | R5448 | R5449 |
| F5071 | L5133 | G5196 | S5260 | K5321 | R5384 | G5449 |
| T5072 | D5134 | G5197 | A5261 | K5322 | A5386 | W5450 |
| G5073 | L5135 | G5198 | T5263 | G5323 | K5389 | F5451 |
| S5074 | P5136 | V5199 | P5264 | L5324 | T5452 | T5452 |
| M5075 | K5137 | A5200 | I5265 | F5325 | F5453 |       |
| G5077 | M5138 | H5201 | E5266 | R5326 | Y5390 |       |
| F5078 | F5139 | H5202 | E5266 | T5327 | F5392 | H5455 |
| S5079 | F5140 | L5203 | F5268 | F5328 | E5393 | A5456 |
| T5080 | L5141 | A5204 | G5269 | P5329 | O5394 | V5457 |
| T5081 | H5142 | A5205 | P5270 | M5330 | O5395 | F5458 |
| G5082 | L5143 | G5206 | T5271 | N5331 | G5396 | A5459 |
| E5083 | A5146 | V5208 | R5272 | K5332 | V5397 | L5460 |
|       | L5147 | G5209 | F5273 | G5333 | T5398 | L5461 |
|       | G5147 | G5210 | Q5274 | D5334 | V5399 | F5462 |
|       | L5148 | L5210 | W5275 |       | S5400 | F5463 |
| D5086 | L5149 |       | D5276 | Q5338 | F5401 | F5464 |
| D5087 | C5150 |       | S5277 | A5339 | Y5402 | G5465 |
| P5088 | F5151 |       | E5278 | W5340 | G5403 | H5466 |
| G5089 | F5152 |       | F5280 | K5341 | I5467 | W5468 |
| F5090 | G5153 |       | Q5281 | G5342 | E5405 | H5469 |
| W5091 | F5154 |       | V5282 | V5345 | N5407 | G5470 |
| S5092 | A5155 |       | E5283 | F5346 | G5408 | A5471 |
| F5093 | F5156 |       | E5284 | R5347 | Q5409 | F5472 |
| E5094 | L5157 |       | R5285 | N5348 | T5410 | L5473 |
| G5095 | A5097 |       | R5286 | K5349 |       | L5474 |
| L5096 | F5159 |       | R5287 | E5350 | D5413 | R5475 |
| L5098 | G5160 |       | V5288 |       | P5414 | D5477 |
| A5099 | L5161 |       | Q5289 | E5353 | P5415 | V5478 |
| H5100 | F5162 |       | A5290 | L5354 | V5416 | F5479 |
| L5101 |       |       | S5291 | F5355 | V5417 | S5480 |
| V5102 | G5165 |       | L5228 | R5357 | K5418 | G5481 |
| S5103 | M5166 |       | A5292 | V5358 | S5419 | I5482 |
| G5105 | W5167 |       | L5229 | R5359 | Y5420 | R5483 |
| L5106 | F5168 |       | M5230 | M5359 | A5421 | P5484 |
| L5107 | S5169 |       | G5232 | P5360 | R5422 | E5485 |
| F5108 | D5170 |       | N5233 | A5361 | K5423 | L5486 |
| L5109 | P5171 |       | I5234 | F5362 | A5424 | S5487 |
| A5110 | Y5172 |       | E5235 | E5363 | F5425 | P5488 |
| A5111 | G5173 |       | F5236 | E5364 | G5426 |       |
| C5112 | L5174 |       | A5301 | S5365 | G5427 |       |
| W5113 | T5175 |       | W5302 | F5366 | E5428 |       |
| H5114 | G5176 |       | S5239 | P5367 | I5429 |       |
| W5115 | S5177 |       | A5304 | V5368 | F5430 |       |
| V5116 | F5178 |       | I5305 | L5369 | E5431 |       |
| V5117 | Q5179 |       | P5306 | L5370 | F5432 |       |
| W5118 | P5180 |       | F5307 | T5371 | D5433 |       |
| D5119 | V5181 |       | K5308 | D5372 | T5434 |       |
| L5120 |       |       | L5309 | K5373 | L5437 |       |
| E5121 | A5248 |       | A5310 | N5374 | N5438 |       |
| L5122 | G5186 |       | F5311 | G5375 |       |       |

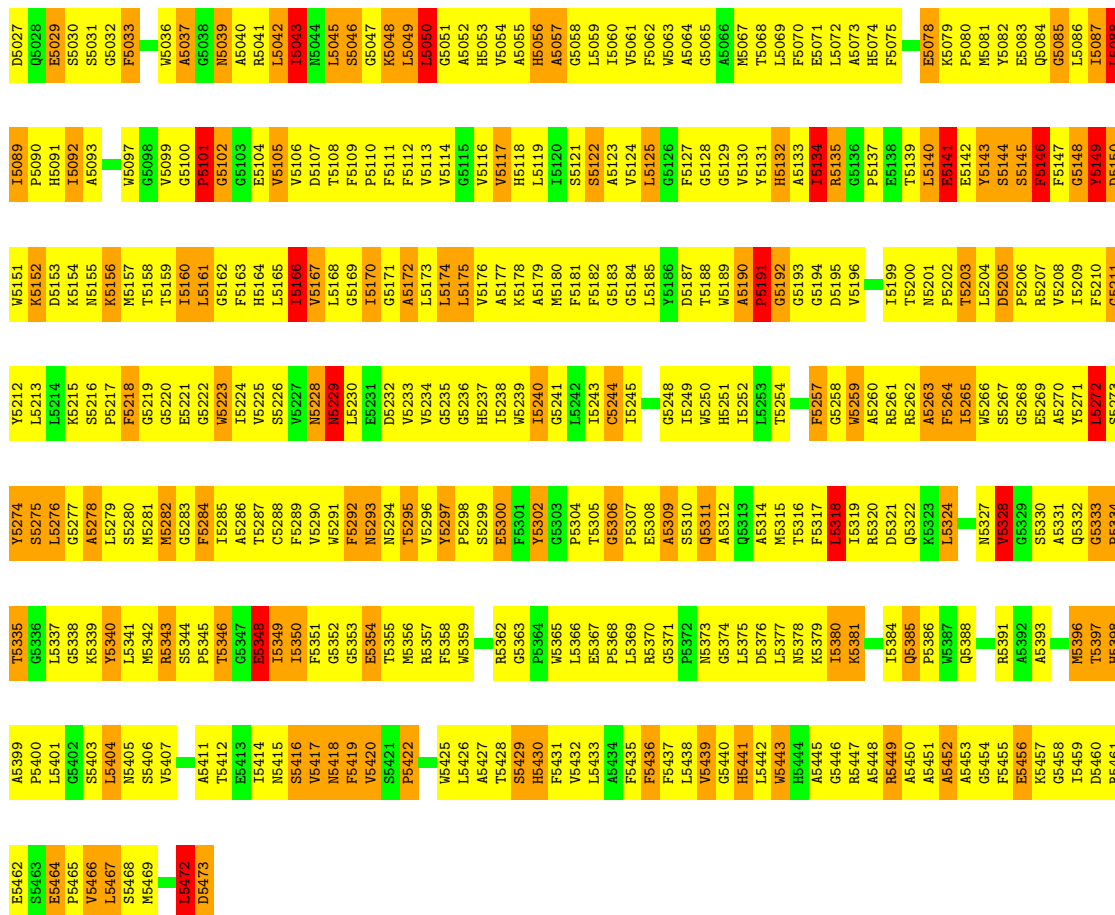
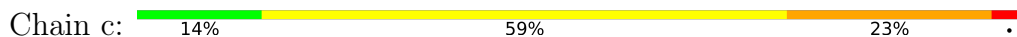
• Molecule 3: Photosystem II CP43 protein



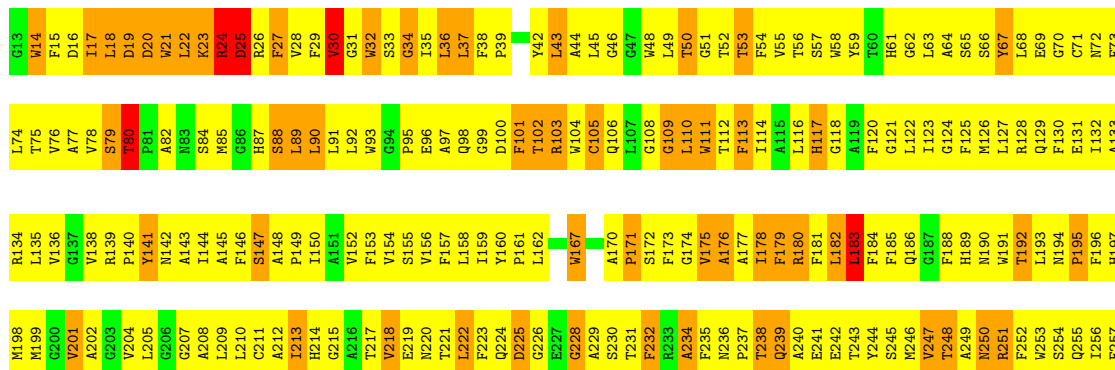
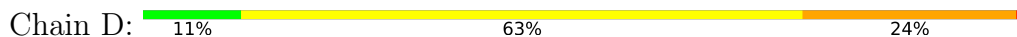
|     |      |      |      |      |      |      |
|-----|------|------|------|------|------|------|
| D27 | I89  | W151 | Y212 | Y274 | T335 | A399 |
| Q28 | P90  | K152 | L213 | S275 | G336 | P400 |
| E29 | H91  | D153 | L214 | L276 | L337 | L401 |
| S30 | I92  | K154 | K215 | G277 | G338 | G402 |
| A93 | A93  | N155 | S216 | A278 | K339 | S403 |
| G32 | K97  | K156 | P217 | L279 | K340 | L404 |
| F33 | G98  | M157 | F218 | S280 | L341 | N405 |
|     | W99  | T158 | G219 | M281 | M342 | N406 |
| W36 | G100 | L159 | G220 | M282 | R343 | N407 |
| A37 | P101 | L160 | E221 | G283 | S344 | G408 |
| G38 | F102 | L161 | G222 | F284 | P345 | G409 |
| N39 | G103 | G162 | W223 | L285 | G346 | V410 |
| A40 | G104 | F163 | L224 | A286 | G347 | A411 |
| R41 | E104 | H164 | V225 | T287 | E348 | T412 |
| L42 | V105 | L165 | S226 | C288 | I349 | E413 |
| L43 | V106 | I166 | V227 | F289 | I350 | E414 |
| N44 | D107 | V167 | N228 | W290 | F351 | N415 |
| L45 | T108 | L168 | N229 | W291 | G352 | S416 |
| S46 | F109 | G169 | L230 | F292 | G353 | V417 |
| G47 | P110 | I170 | E231 | N293 | E354 | N418 |
| K48 | F111 | G171 | D232 | N294 | T355 | F419 |
| L49 | F112 | A172 | V233 | T295 | M356 | V420 |
| L50 | V113 | L173 | V234 | V296 | R357 | S421 |
| G51 | V114 | L174 | G235 | Y297 | F358 | P422 |
| A52 | G115 | L175 | G236 | P298 | W359 |      |
| H53 | V116 | V176 | H237 | S299 |      | W425 |
| V54 | V117 | A177 | L238 | E300 | R362 | L426 |
| A55 | H118 | K178 | W239 | F301 | G363 | A427 |
| H56 | L119 | A179 | L240 | Y302 | P364 | T428 |
| A57 | N120 | M180 | G241 | G303 | V365 | S429 |
| G58 | S121 | F181 | L242 | P304 | L366 | H430 |
| L59 | S122 | F182 | L243 | T305 | E367 | F431 |
| L60 | A123 | G183 | G244 | G306 | P368 | V432 |
| V61 | V124 | G184 | L245 | P307 | L369 | L433 |
| F62 | L125 | L185 |      | E308 | R370 | A434 |
| W63 | G126 | Y186 | G248 | A309 | G371 | F435 |
| A64 | F127 | D187 | L249 | S310 | P372 | F436 |
| G65 | G128 | T188 | V250 | Q311 | N373 | F437 |
| A66 | G129 | W189 | H251 | A312 | G374 | L438 |
| M67 | V130 | A190 | L252 | Q313 | L375 | V439 |
| T68 | Y131 | P191 | L253 | A314 | D376 | G440 |
| L69 | H132 | G192 | T254 | M315 | L377 | H441 |
| F70 | A133 | G193 |      | T316 | K378 | L442 |
| E71 | I134 | G194 | F257 | F317 | K379 | W443 |
| L72 | R135 | D195 | G258 | L318 | I380 | H444 |
| H74 | P137 | V196 | W259 | I319 | A445 | A445 |
| F75 | G138 | T199 | A260 | R320 | G446 | G446 |
| E78 | L140 | N201 | R261 | D321 | R447 | A448 |
| K79 | E141 | T202 | A263 | Q322 | R449 | R449 |
| P80 | L142 | P203 | F264 | K323 | L324 | A450 |
| M81 | Y143 | T204 | W266 | N327 |      | A451 |
| Y82 | S144 | D205 | S267 | V328 |      | A452 |
| E83 | S145 | G268 | G268 | G329 |      | A453 |
| O84 | F146 | R207 | E269 | A392 |      | G454 |
| G85 | F147 | V208 | A270 | A393 |      | F455 |
| L86 | G148 | T209 | L271 | E456 |      | E456 |
| L87 | Y149 | G211 | S273 | K457 |      | K457 |
| L88 | D150 |      |      | T397 |      | G458 |

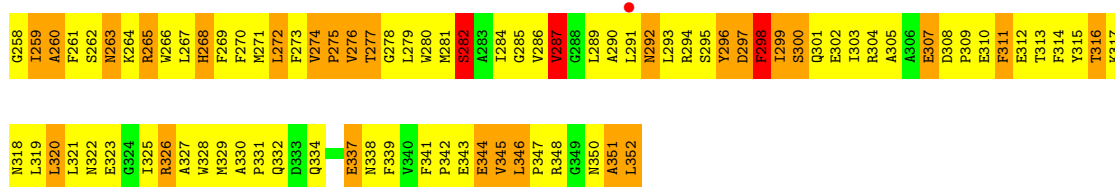


- Molecule 3: Photosystem II CP43 protein



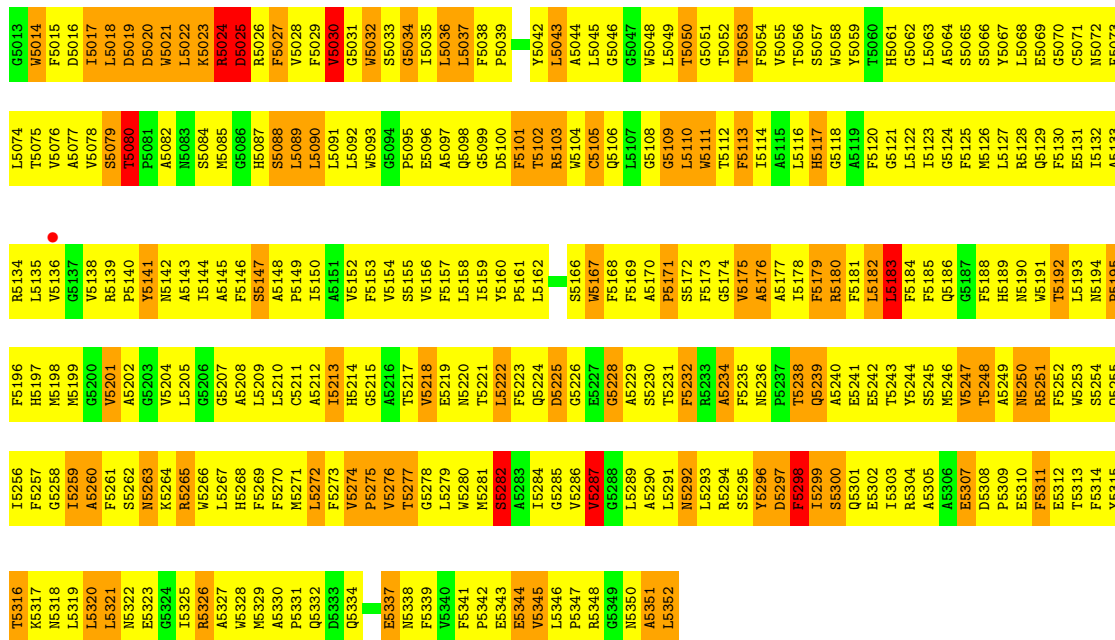
- Molecule 4: Photosystem II D2 protein





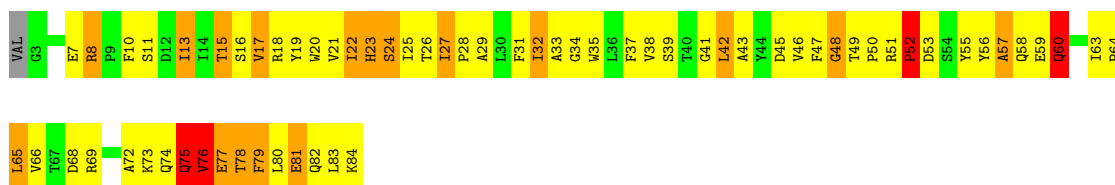
### • Molecule 4: Photosystem II D2 protein

Chain d: 10% 64% 23%



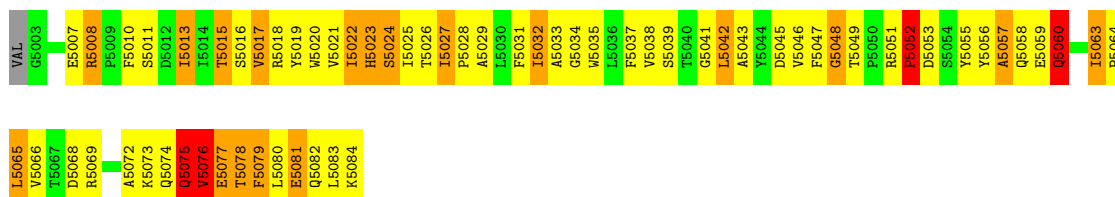
### • Molecule 5: Cytochrome b559 subunit alpha

Chain E: 20% 53% 20% 5%

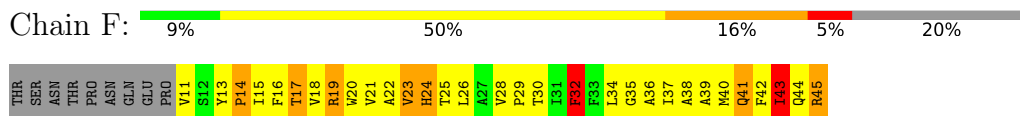


### • Molecule 5: Cytochrome b559 subunit alpha

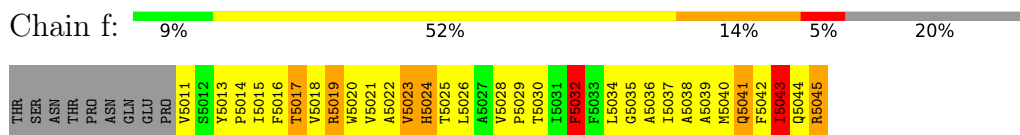
Chain e: 22% 51% 22% 5%



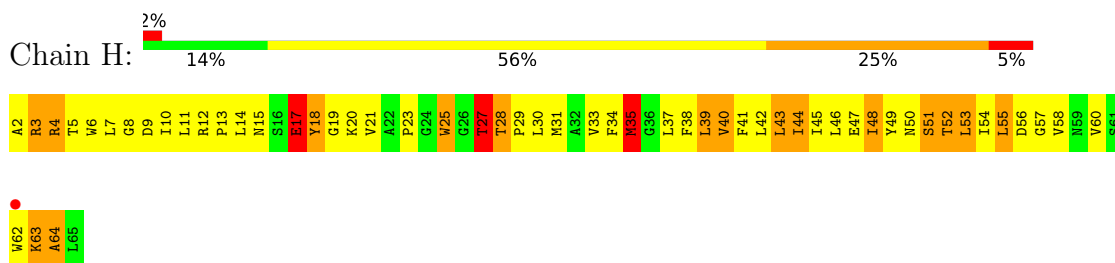
- Molecule 6: Cytochrome b559 subunit beta



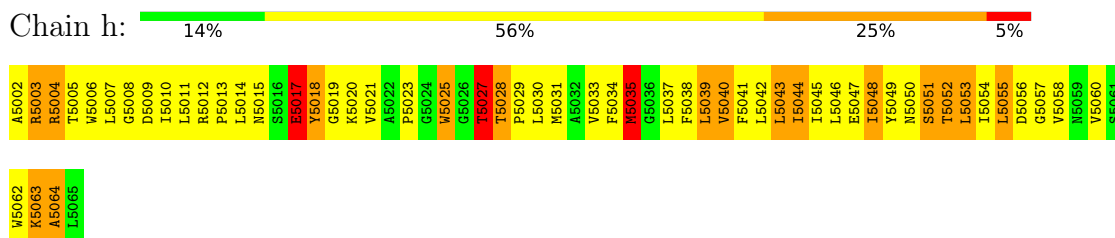
- Molecule 6: Cytochrome b559 subunit beta



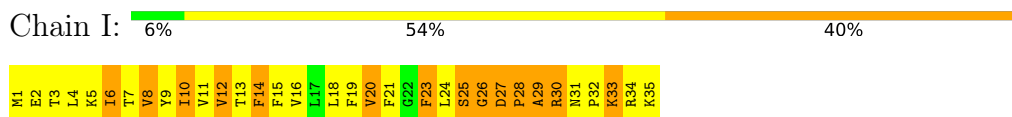
- Molecule 7: Photosystem II reaction center protein H



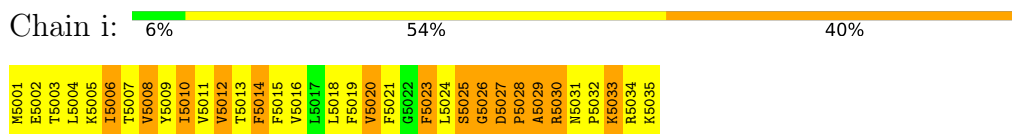
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



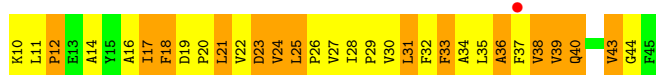
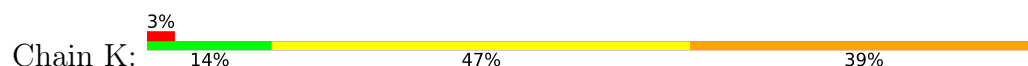




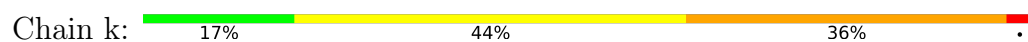
- Molecule 9: Photosystem II reaction center protein J



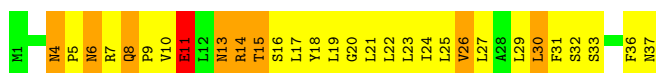
- Molecule 10: Photosystem II reaction center protein K



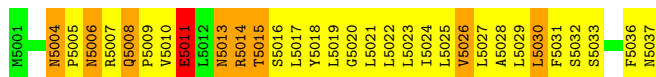
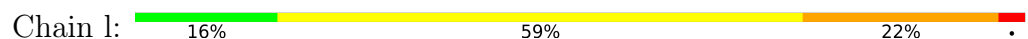
- Molecule 10: Photosystem II reaction center protein K



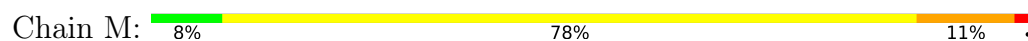
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



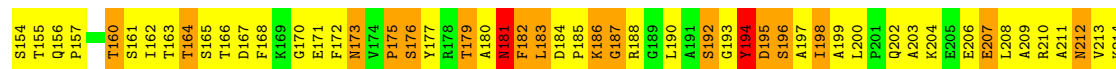
- Molecule 12: Photosystem II reaction center protein M





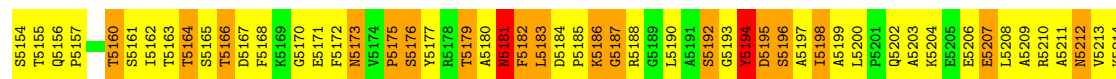
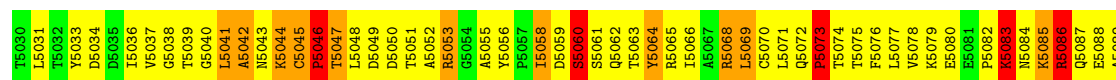
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 20% 55% 21%



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 20% 55% 21%



• Molecule 14: Photosystem II reaction center protein T

Chain T: 10% 67% 20%

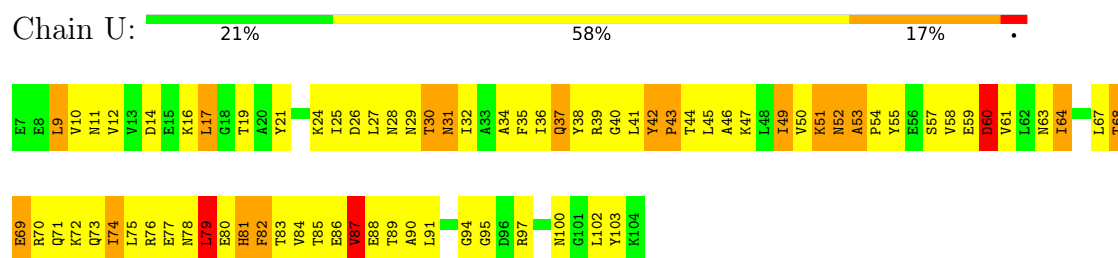


• Molecule 14: Photosystem II reaction center protein T

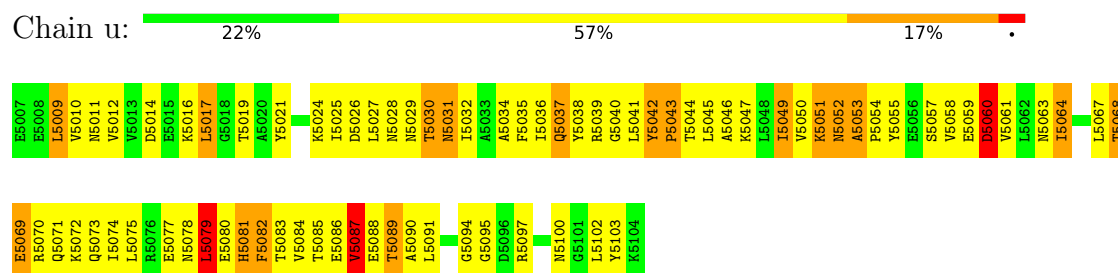
Chain t: 13% 63% 17% 7%



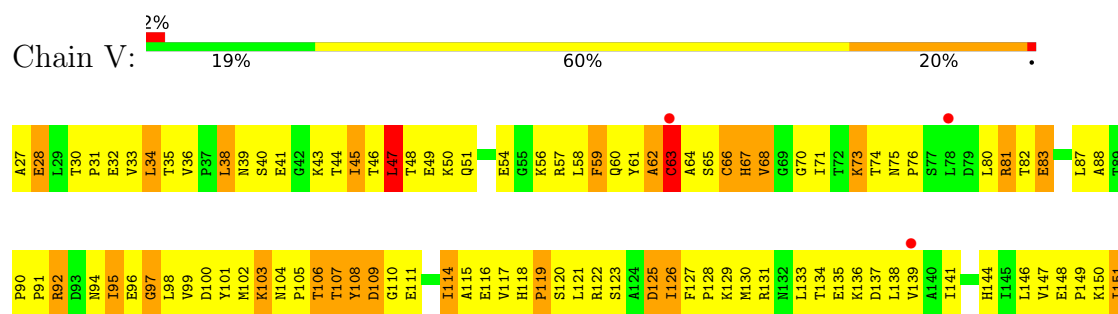
- Molecule 15: Photosystem II 12 kDa extrinsic protein



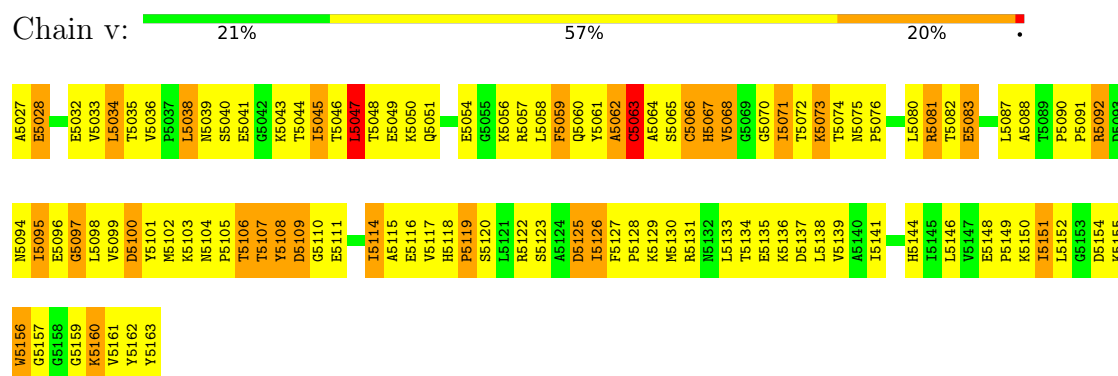
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



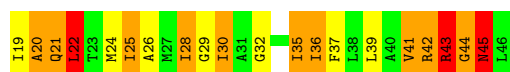
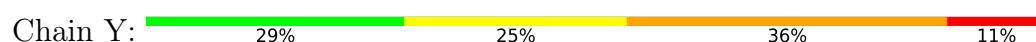
- Molecule 17: Photosystem II reaction center protein X



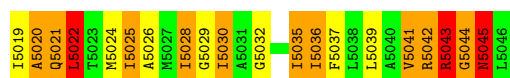
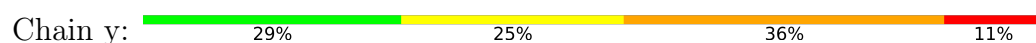
- Molecule 17: Photosystem II reaction center protein X



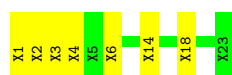
- Molecule 18: Photosystem II reaction center protein ycf12



- Molecule 18: Photosystem II reaction center protein ycf12



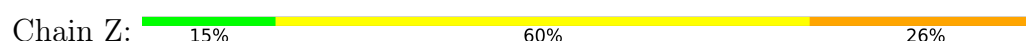
- Molecule 19: Photosystem II reaction center protein Y



- Molecule 19: Photosystem II reaction center protein Y

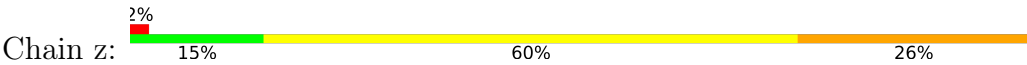


- Molecule 20: Photosystem II reaction center protein Z



V62

• Molecule 20: Photosystem II reaction center protein Z



V5061  
V5062

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 128.50Å 224.70Å 304.92Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 4.00<br>20.00 – 4.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.7 (20.00-4.00)<br>93.9 (20.00-4.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.08 (at 4.07Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.290 , 0.326<br>0.278 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3592 reflections (5.08%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 148.7                                                       | Xtriage          |
| Anisotropy                                                              | 0.518                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.23 , 71.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 48060                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 165.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, HEM, DGD, FE2, CLA, PQ9, LHG, MGE, BCR, OEC, PHO

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$   | RMSZ        | # $ Z  > 5$    |
| 1   | A     | 0.66         | 0/2714        | 1.19        | 38/3699 (1.0%) |
| 1   | a     | 0.66         | 0/2714        | 1.19        | 37/3699 (1.0%) |
| 2   | B     | 0.68         | 0/3971        | 1.27        | 59/5411 (1.1%) |
| 2   | b     | 0.68         | 0/3971        | 1.27        | 59/5411 (1.1%) |
| 3   | C     | 0.62         | 1/3568 (0.0%) | 1.28        | 52/4858 (1.1%) |
| 3   | c     | 0.63         | 1/3568 (0.0%) | 1.28        | 52/4858 (1.1%) |
| 4   | D     | 0.65         | 0/2801        | 1.22        | 34/3818 (0.9%) |
| 4   | d     | 0.65         | 0/2801        | 1.22        | 33/3818 (0.9%) |
| 5   | E     | 0.66         | 0/685         | 1.32        | 7/933 (0.8%)   |
| 5   | e     | 0.66         | 0/685         | 1.32        | 7/933 (0.8%)   |
| 6   | F     | 0.69         | 0/291         | 1.07        | 1/397 (0.3%)   |
| 6   | f     | 0.69         | 0/291         | 1.07        | 1/397 (0.3%)   |
| 7   | H     | 0.70         | 1/520 (0.2%)  | 1.27        | 8/708 (1.1%)   |
| 7   | h     | 0.70         | 1/520 (0.2%)  | 1.27        | 8/708 (1.1%)   |
| 8   | I     | 0.80         | 0/294         | 1.07        | 2/395 (0.5%)   |
| 8   | i     | 0.80         | 0/294         | 1.07        | 2/395 (0.5%)   |
| 9   | J     | 0.78         | 0/255         | 1.22        | 2/346 (0.6%)   |
| 9   | j     | 0.78         | 0/255         | 1.22        | 2/346 (0.6%)   |
| 10  | K     | 0.66         | 0/287         | 1.25        | 2/394 (0.5%)   |
| 10  | k     | 0.66         | 0/287         | 1.27        | 3/394 (0.8%)   |
| 11  | L     | 0.69         | 0/311         | 1.12        | 3/422 (0.7%)   |
| 11  | l     | 0.69         | 0/311         | 1.11        | 3/422 (0.7%)   |
| 12  | M     | 0.70         | 0/287         | 1.10        | 3/388 (0.8%)   |
| 12  | m     | 0.70         | 0/287         | 1.09        | 3/388 (0.8%)   |
| 13  | O     | 0.66         | 0/1891        | 1.24        | 23/2564 (0.9%) |
| 13  | o     | 0.66         | 0/1891        | 1.24        | 23/2564 (0.9%) |
| 14  | T     | 0.77         | 0/266         | 1.47        | 7/359 (1.9%)   |
| 14  | t     | 0.74         | 0/266         | 1.45        | 7/359 (1.9%)   |
| 15  | U     | 0.60         | 0/794         | 1.19        | 8/1076 (0.7%)  |
| 15  | u     | 0.59         | 0/794         | 1.18        | 8/1076 (0.7%)  |
| 16  | V     | 0.58         | 0/1085        | 1.18        | 13/1473 (0.9%) |
| 16  | v     | 0.58         | 0/1085        | 1.18        | 13/1473 (0.9%) |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 17  | X     | 0.62         | 0/249          | 1.16        | 0/337            |
| 17  | x     | 0.62         | 0/249          | 1.16        | 0/337            |
| 18  | Y     | 0.84         | 0/209          | 1.35        | 1/279 (0.4%)     |
| 18  | y     | 0.84         | 0/209          | 1.35        | 1/279 (0.4%)     |
| 20  | Z     | 0.64         | 0/490          | 1.19        | 6/669 (0.9%)     |
| 20  | z     | 0.64         | 0/490          | 1.19        | 6/669 (0.9%)     |
| All | All   | 0.66         | 4/41936 (0.0%) | 1.24        | 537/57052 (0.9%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | c     | 5346 | THR  | CA-CB | 5.83 | 1.60        | 1.53     |
| 3   | C     | 346  | THR  | CA-CB | 5.81 | 1.60        | 1.53     |
| 7   | h     | 5035 | MET  | SD-CE | 5.24 | 1.92        | 1.79     |
| 7   | H     | 35   | MET  | SD-CE | 5.23 | 1.92        | 1.79     |

All (537) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 2   | B     | 170  | ASP  | CA-C-N | 15.15  | 138.78      | 119.84   |
| 2   | B     | 170  | ASP  | C-N-CA | 15.15  | 138.78      | 119.84   |
| 2   | b     | 5170 | ASP  | CA-C-N | 15.15  | 138.78      | 119.84   |
| 2   | b     | 5170 | ASP  | C-N-CA | 15.15  | 138.78      | 119.84   |
| 3   | c     | 5050 | LEU  | N-CA-C | -12.24 | 97.93       | 111.28   |
| 3   | C     | 50   | LEU  | N-CA-C | -12.22 | 97.96       | 111.28   |
| 3   | c     | 5354 | GLU  | N-CA-C | -11.78 | 97.74       | 114.12   |
| 3   | C     | 354  | GLU  | N-CA-C | -11.78 | 97.75       | 114.12   |
| 16  | V     | 110  | GLY  | N-CA-C | -11.41 | 99.44       | 115.30   |
| 16  | v     | 5110 | GLY  | N-CA-C | -11.37 | 99.49       | 115.30   |
| 4   | d     | 5296 | TYR  | N-CA-C | -10.55 | 98.90       | 112.93   |
| 4   | D     | 296  | TYR  | N-CA-C | -10.53 | 98.93       | 112.93   |
| 1   | A     | 33   | PHE  | N-CA-C | -10.35 | 99.96       | 111.14   |
| 1   | a     | 5033 | PHE  | N-CA-C | -10.34 | 99.97       | 111.14   |
| 14  | T     | 4    | ILE  | N-CA-C | -10.16 | 100.81      | 111.58   |
| 14  | t     | 5004 | ILE  | N-CA-C | -10.15 | 100.82      | 111.58   |
| 3   | c     | 5349 | ILE  | N-CA-C | 10.07  | 122.20      | 108.11   |
| 3   | C     | 349  | ILE  | N-CA-C | 10.05  | 122.18      | 108.11   |
| 4   | d     | 5080 | THR  | CA-C-N | 9.85   | 130.47      | 119.93   |
| 4   | d     | 5080 | THR  | C-N-CA | 9.85   | 130.47      | 119.93   |
| 4   | D     | 80   | THR  | CA-C-N | 9.82   | 130.44      | 119.93   |
| 4   | D     | 80   | THR  | C-N-CA | 9.82   | 130.44      | 119.93   |
| 13  | o     | 5196 | SER  | N-CA-C | 9.57   | 120.87      | 108.24   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 13  | O     | 196  | SER  | N-CA-C | 9.52  | 120.81      | 108.24   |
| 1   | A     | 335  | ASN  | N-CA-C | 9.50  | 121.64      | 111.28   |
| 1   | a     | 5335 | ASN  | N-CA-C | 9.47  | 121.60      | 111.28   |
| 4   | D     | 239  | GLN  | N-CA-C | 9.44  | 122.58      | 109.18   |
| 4   | d     | 5239 | GLN  | N-CA-C | 9.44  | 122.58      | 109.18   |
| 5   | E     | 8    | ARG  | CA-C-N | 9.18  | 129.25      | 119.89   |
| 5   | E     | 8    | ARG  | C-N-CA | 9.18  | 129.25      | 119.89   |
| 2   | b     | 5005 | TRP  | N-CA-C | 9.15  | 122.09      | 111.11   |
| 2   | B     | 5    | TRP  | N-CA-C | 9.15  | 122.09      | 111.11   |
| 5   | e     | 5008 | ARG  | CA-C-N | 9.14  | 129.21      | 119.89   |
| 5   | e     | 5008 | ARG  | C-N-CA | 9.14  | 129.21      | 119.89   |
| 13  | o     | 5045 | CYS  | CA-C-N | 9.07  | 131.17      | 119.84   |
| 13  | o     | 5045 | CYS  | C-N-CA | 9.07  | 131.17      | 119.84   |
| 13  | O     | 45   | CYS  | CA-C-N | 9.05  | 131.15      | 119.84   |
| 13  | O     | 45   | CYS  | C-N-CA | 9.05  | 131.15      | 119.84   |
| 3   | C     | 278  | ALA  | N-CA-C | -8.93 | 102.52      | 113.50   |
| 3   | c     | 5278 | ALA  | N-CA-C | -8.92 | 102.53      | 113.50   |
| 13  | o     | 5187 | GLY  | N-CA-C | 8.92  | 126.75      | 115.42   |
| 3   | c     | 5297 | TYR  | CA-C-N | 8.90  | 130.97      | 119.84   |
| 3   | c     | 5297 | TYR  | C-N-CA | 8.90  | 130.97      | 119.84   |
| 13  | O     | 187  | GLY  | N-CA-C | 8.88  | 126.70      | 115.42   |
| 3   | C     | 297  | TYR  | CA-C-N | 8.88  | 130.94      | 119.84   |
| 3   | C     | 297  | TYR  | C-N-CA | 8.88  | 130.94      | 119.84   |
| 1   | A     | 76   | ASN  | N-CA-C | -8.82 | 97.80       | 110.59   |
| 1   | a     | 5076 | ASN  | N-CA-C | -8.81 | 97.82       | 110.59   |
| 3   | c     | 5318 | LEU  | N-CA-C | -8.49 | 102.02      | 111.28   |
| 3   | C     | 318  | LEU  | N-CA-C | -8.48 | 102.04      | 111.28   |
| 2   | B     | 73   | GLY  | N-CA-C | 8.46  | 123.50      | 111.14   |
| 2   | b     | 5073 | GLY  | N-CA-C | 8.45  | 123.48      | 111.14   |
| 9   | j     | 5030 | TYR  | N-CA-C | -8.30 | 101.92      | 110.97   |
| 4   | D     | 334  | GLN  | CA-C-N | 8.29  | 128.26      | 119.05   |
| 4   | D     | 334  | GLN  | C-N-CA | 8.29  | 128.26      | 119.05   |
| 9   | J     | 30   | TYR  | N-CA-C | -8.29 | 101.94      | 110.97   |
| 3   | c     | 5172 | ALA  | N-CA-C | -8.28 | 101.31      | 111.33   |
| 4   | d     | 5334 | GLN  | CA-C-N | 8.28  | 128.24      | 119.05   |
| 4   | d     | 5334 | GLN  | C-N-CA | 8.28  | 128.24      | 119.05   |
| 3   | C     | 172  | ALA  | N-CA-C | -8.28 | 101.31      | 111.33   |
| 13  | o     | 5102 | THR  | N-CA-C | 8.26  | 123.93      | 112.04   |
| 13  | O     | 102  | THR  | N-CA-C | 8.25  | 123.92      | 112.04   |
| 2   | B     | 26   | HIS  | N-CA-C | -8.25 | 101.62      | 112.34   |
| 2   | b     | 5026 | HIS  | N-CA-C | -8.25 | 101.62      | 112.34   |
| 3   | C     | 149  | TYR  | N-CA-C | 8.22  | 123.04      | 109.06   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 15  | U     | 17   | LEU  | N-CA-C | -8.22 | 103.24      | 113.18   |
| 15  | u     | 5017 | LEU  | N-CA-C | -8.21 | 103.24      | 113.18   |
| 3   | c     | 5149 | TYR  | N-CA-C | 8.21  | 123.01      | 109.06   |
| 7   | H     | 57   | GLY  | N-CA-C | -8.20 | 102.39      | 114.61   |
| 7   | h     | 5057 | GLY  | N-CA-C | -8.19 | 102.40      | 114.61   |
| 4   | d     | 5147 | SER  | N-CA-C | -8.13 | 102.42      | 111.28   |
| 4   | D     | 147  | SER  | N-CA-C | -8.12 | 102.43      | 111.28   |
| 13  | O     | 90   | GLU  | N-CA-C | 8.10  | 122.98      | 110.42   |
| 13  | o     | 5090 | GLU  | N-CA-C | 8.10  | 122.97      | 110.42   |
| 13  | o     | 5040 | GLY  | N-CA-C | -8.06 | 101.09      | 114.48   |
| 13  | O     | 40   | GLY  | N-CA-C | -8.06 | 101.11      | 114.48   |
| 2   | B     | 381  | ILE  | CA-C-N | 7.96  | 128.01      | 119.89   |
| 2   | B     | 381  | ILE  | C-N-CA | 7.96  | 128.01      | 119.89   |
| 2   | b     | 5381 | ILE  | CA-C-N | 7.96  | 128.01      | 119.89   |
| 2   | b     | 5381 | ILE  | C-N-CA | 7.96  | 128.01      | 119.89   |
| 1   | A     | 296  | ASN  | N-CA-C | 7.91  | 122.59      | 111.52   |
| 1   | a     | 5296 | ASN  | N-CA-C | 7.89  | 122.56      | 111.52   |
| 13  | O     | 181  | ASN  | N-CA-C | -7.84 | 100.42      | 110.53   |
| 13  | o     | 5181 | ASN  | N-CA-C | -7.82 | 100.44      | 110.53   |
| 16  | V     | 62   | ALA  | N-CA-C | -7.81 | 103.63      | 113.01   |
| 10  | K     | 18   | PHE  | N-CA-C | 7.81  | 123.01      | 113.17   |
| 10  | k     | 5018 | PHE  | N-CA-C | 7.81  | 123.01      | 113.17   |
| 14  | t     | 5016 | LEU  | N-CA-C | -7.81 | 103.73      | 113.18   |
| 3   | C     | 166  | ILE  | N-CA-C | -7.79 | 102.68      | 110.62   |
| 16  | v     | 5062 | ALA  | N-CA-C | -7.79 | 103.66      | 113.01   |
| 3   | c     | 5166 | ILE  | N-CA-C | -7.79 | 102.68      | 110.62   |
| 14  | T     | 16   | LEU  | N-CA-C | -7.78 | 103.77      | 113.18   |
| 3   | c     | 5311 | GLN  | N-CA-C | -7.76 | 103.78      | 113.55   |
| 3   | C     | 311  | GLN  | N-CA-C | -7.74 | 103.80      | 113.55   |
| 3   | c     | 5300 | GLU  | N-CA-C | -7.73 | 103.83      | 113.18   |
| 3   | C     | 293  | ASN  | N-CA-C | 7.71  | 122.40      | 109.76   |
| 3   | C     | 300  | GLU  | N-CA-C | -7.69 | 103.87      | 113.18   |
| 3   | c     | 5293 | ASN  | N-CA-C | 7.68  | 122.36      | 109.76   |
| 2   | B     | 349  | LYS  | N-CA-C | -7.64 | 102.89      | 112.90   |
| 2   | b     | 5349 | LYS  | N-CA-C | -7.62 | 102.91      | 112.90   |
| 2   | b     | 5327 | THR  | N-CA-C | 7.59  | 126.96      | 110.80   |
| 2   | B     | 327  | THR  | N-CA-C | 7.56  | 126.91      | 110.80   |
| 10  | K     | 24   | VAL  | N-CA-C | 7.56  | 119.24      | 111.00   |
| 10  | k     | 5024 | VAL  | N-CA-C | 7.55  | 119.23      | 111.00   |
| 2   | b     | 5110 | ALA  | N-CA-C | -7.55 | 102.08      | 111.75   |
| 2   | B     | 110  | ALA  | N-CA-C | -7.54 | 102.09      | 111.75   |
| 2   | b     | 5310 | ALA  | N-CA-C | -7.47 | 102.83      | 110.97   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | B     | 310  | ALA  | N-CA-C | -7.45 | 102.85      | 110.97   |
| 5   | e     | 5023 | HIS  | N-CA-C | 7.41  | 119.14      | 111.14   |
| 5   | E     | 23   | HIS  | N-CA-C | 7.40  | 119.13      | 111.14   |
| 4   | d     | 5346 | LEU  | CA-C-N | 7.34  | 127.61      | 119.90   |
| 4   | d     | 5346 | LEU  | C-N-CA | 7.34  | 127.61      | 119.90   |
| 4   | D     | 346  | LEU  | CA-C-N | 7.33  | 127.60      | 119.90   |
| 4   | D     | 346  | LEU  | C-N-CA | 7.33  | 127.60      | 119.90   |
| 13  | O     | 217  | SER  | N-CA-C | 7.32  | 120.20      | 110.53   |
| 3   | C     | 37   | ALA  | N-CA-C | -7.31 | 104.31      | 112.57   |
| 3   | c     | 5037 | ALA  | N-CA-C | -7.29 | 104.33      | 112.57   |
| 3   | C     | 284  | PHE  | N-CA-C | -7.28 | 103.28      | 111.07   |
| 13  | o     | 5217 | SER  | N-CA-C | 7.28  | 120.14      | 110.53   |
| 3   | c     | 5284 | PHE  | N-CA-C | -7.28 | 103.28      | 111.07   |
| 3   | C     | 148  | GLY  | N-CA-C | 7.26  | 124.86      | 112.22   |
| 3   | c     | 5148 | GLY  | N-CA-C | 7.25  | 124.84      | 112.22   |
| 3   | c     | 5292 | PHE  | N-CA-C | 7.24  | 122.79      | 113.88   |
| 4   | D     | 238  | THR  | N-CA-C | 7.23  | 119.06      | 111.03   |
| 3   | C     | 292  | PHE  | N-CA-C | 7.23  | 122.78      | 113.88   |
| 3   | c     | 5396 | MET  | N-CA-C | -7.20 | 103.37      | 111.14   |
| 1   | A     | 320  | ILE  | N-CA-C | -7.18 | 103.78      | 110.53   |
| 3   | C     | 396  | MET  | N-CA-C | -7.18 | 103.38      | 111.14   |
| 4   | d     | 5238 | THR  | N-CA-C | 7.18  | 119.00      | 111.03   |
| 1   | a     | 5320 | ILE  | N-CA-C | -7.17 | 103.79      | 110.53   |
| 1   | A     | 229  | GLU  | N-CA-C | -7.16 | 104.81      | 113.97   |
| 1   | a     | 5229 | GLU  | N-CA-C | -7.15 | 104.81      | 113.97   |
| 11  | l     | 5011 | GLU  | N-CA-C | 7.13  | 120.81      | 108.76   |
| 2   | b     | 5366 | PHE  | CA-C-N | 7.12  | 128.75      | 119.84   |
| 2   | b     | 5366 | PHE  | C-N-CA | 7.12  | 128.75      | 119.84   |
| 11  | L     | 11   | GLU  | N-CA-C | 7.12  | 120.79      | 108.76   |
| 2   | B     | 366  | PHE  | CA-C-N | 7.11  | 128.72      | 119.84   |
| 2   | B     | 366  | PHE  | C-N-CA | 7.11  | 128.72      | 119.84   |
| 1   | A     | 126  | TYR  | N-CA-C | -7.10 | 103.62      | 111.36   |
| 1   | a     | 5126 | TYR  | N-CA-C | -7.10 | 103.62      | 111.36   |
| 15  | U     | 12   | VAL  | N-CA-C | 7.08  | 118.72      | 111.00   |
| 1   | a     | 5277 | ALA  | N-CA-C | 7.08  | 119.89      | 111.33   |
| 2   | b     | 5384 | ARG  | N-CA-C | -7.08 | 103.50      | 111.14   |
| 15  | u     | 5012 | VAL  | N-CA-C | 7.07  | 118.71      | 111.00   |
| 1   | A     | 277  | ALA  | N-CA-C | 7.07  | 119.88      | 111.33   |
| 2   | B     | 384  | ARG  | N-CA-C | -7.06 | 103.52      | 111.14   |
| 20  | z     | 5054 | VAL  | N-CA-C | -7.05 | 101.74      | 111.89   |
| 20  | Z     | 54   | VAL  | N-CA-C | -7.03 | 101.76      | 111.89   |
| 4   | D     | 287  | VAL  | N-CA-C | -7.02 | 102.61      | 110.62   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | d     | 5287 | VAL  | N-CA-C | -7.02 | 102.62      | 110.62   |
| 2   | B     | 364  | GLU  | N-CA-C | -7.00 | 103.73      | 112.90   |
| 2   | B     | 221  | PRO  | N-CA-C | 6.98  | 119.21      | 110.70   |
| 2   | b     | 5364 | GLU  | N-CA-C | -6.97 | 103.76      | 112.90   |
| 2   | b     | 5221 | PRO  | N-CA-C | 6.96  | 119.19      | 110.70   |
| 3   | C     | 348  | GLU  | N-CA-C | 6.95  | 118.86      | 111.28   |
| 3   | c     | 5348 | GLU  | N-CA-C | 6.94  | 118.84      | 111.28   |
| 16  | v     | 5122 | ARG  | N-CA-C | -6.91 | 103.75      | 111.28   |
| 16  | V     | 122  | ARG  | N-CA-C | -6.88 | 103.78      | 111.28   |
| 2   | b     | 5405 | GLU  | N-CA-C | -6.87 | 105.45      | 114.31   |
| 4   | D     | 24   | ARG  | N-CA-C | 6.86  | 120.85      | 109.46   |
| 2   | B     | 405  | GLU  | N-CA-C | -6.85 | 105.47      | 114.31   |
| 1   | A     | 331  | MET  | N-CA-C | 6.85  | 118.44      | 110.97   |
| 4   | d     | 5024 | ARG  | N-CA-C | 6.84  | 120.81      | 109.46   |
| 1   | a     | 5331 | MET  | N-CA-C | 6.82  | 118.41      | 110.97   |
| 2   | b     | 5172 | TYR  | N-CA-C | -6.82 | 99.04       | 109.41   |
| 2   | B     | 172  | TYR  | N-CA-C | -6.81 | 99.06       | 109.41   |
| 20  | Z     | 33   | TRP  | N-CA-C | -6.79 | 103.94      | 111.82   |
| 20  | z     | 5033 | TRP  | N-CA-C | -6.78 | 103.96      | 111.82   |
| 3   | C     | 143  | TYR  | N-CA-C | -6.77 | 104.12      | 112.38   |
| 3   | c     | 5143 | TYR  | N-CA-C | -6.74 | 104.15      | 112.38   |
| 20  | Z     | 17   | PHE  | N-CA-C | -6.74 | 103.93      | 111.28   |
| 20  | z     | 5017 | PHE  | N-CA-C | -6.74 | 103.93      | 111.28   |
| 1   | A     | 266  | ASN  | N-CA-C | -6.71 | 105.38      | 113.97   |
| 1   | a     | 5266 | ASN  | N-CA-C | -6.70 | 105.39      | 113.97   |
| 2   | b     | 5332 | LYS  | N-CA-C | -6.67 | 104.12      | 113.20   |
| 9   | J     | 34   | ALA  | N-CA-C | -6.66 | 105.44      | 113.97   |
| 18  | y     | 5022 | LEU  | N-CA-C | 6.66  | 118.19      | 111.07   |
| 2   | B     | 332  | LYS  | N-CA-C | -6.65 | 104.16      | 113.20   |
| 4   | d     | 5175 | VAL  | N-CA-C | -6.65 | 105.36      | 111.67   |
| 3   | c     | 5263 | ALA  | N-CA-C | 6.63  | 118.39      | 111.03   |
| 3   | C     | 263  | ALA  | N-CA-C | 6.63  | 118.39      | 111.03   |
| 18  | Y     | 22   | LEU  | N-CA-C | 6.62  | 118.16      | 111.07   |
| 9   | j     | 5034 | ALA  | N-CA-C | -6.62 | 105.50      | 113.97   |
| 4   | D     | 175  | VAL  | N-CA-C | -6.61 | 105.39      | 111.67   |
| 7   | h     | 5023 | PRO  | N-CA-C | 6.61  | 120.78      | 110.80   |
| 7   | H     | 23   | PRO  | N-CA-C | 6.60  | 120.77      | 110.80   |
| 7   | H     | 63   | LYS  | N-CA-C | -6.57 | 100.56      | 110.28   |
| 3   | c     | 5464 | GLU  | CA-C-N | 6.55  | 126.79      | 119.32   |
| 3   | c     | 5464 | GLU  | C-N-CA | 6.55  | 126.79      | 119.32   |
| 7   | h     | 5063 | LYS  | N-CA-C | -6.54 | 100.61      | 110.28   |
| 1   | a     | 5195 | HIS  | CA-C-N | 6.53  | 128.00      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | a     | 5195 | HIS  | C-N-CA | 6.53  | 128.00      | 119.84   |
| 3   | C     | 114  | VAL  | N-CA-C | 6.52  | 118.05      | 110.62   |
| 3   | c     | 5218 | PHE  | N-CA-C | 6.52  | 119.35      | 110.35   |
| 3   | C     | 218  | PHE  | N-CA-C | 6.52  | 119.34      | 110.35   |
| 3   | C     | 439  | VAL  | N-CA-C | -6.52 | 103.97      | 110.62   |
| 1   | A     | 195  | HIS  | CA-C-N | 6.51  | 127.97      | 119.84   |
| 1   | A     | 195  | HIS  | C-N-CA | 6.51  | 127.97      | 119.84   |
| 3   | C     | 464  | GLU  | CA-C-N | 6.50  | 126.73      | 119.32   |
| 3   | C     | 464  | GLU  | C-N-CA | 6.50  | 126.73      | 119.32   |
| 2   | b     | 5372 | ASP  | N-CA-C | -6.50 | 101.51      | 110.35   |
| 16  | V     | 33   | VAL  | N-CA-C | -6.50 | 104.55      | 113.00   |
| 3   | c     | 5439 | VAL  | N-CA-C | -6.50 | 103.99      | 110.62   |
| 3   | c     | 5114 | VAL  | N-CA-C | 6.49  | 118.02      | 110.62   |
| 2   | B     | 372  | ASP  | N-CA-C | -6.48 | 101.53      | 110.35   |
| 1   | A     | 83   | VAL  | CA-C-N | 6.47  | 127.92      | 119.84   |
| 1   | A     | 83   | VAL  | C-N-CA | 6.47  | 127.92      | 119.84   |
| 16  | v     | 5033 | VAL  | N-CA-C | -6.46 | 104.60      | 113.00   |
| 1   | a     | 5036 | ILE  | N-CA-C | -6.45 | 106.01      | 111.56   |
| 1   | a     | 5083 | VAL  | CA-C-N | 6.45  | 127.90      | 119.84   |
| 1   | a     | 5083 | VAL  | C-N-CA | 6.45  | 127.90      | 119.84   |
| 1   | A     | 36   | ILE  | N-CA-C | -6.44 | 106.02      | 111.56   |
| 13  | O     | 208  | LEU  | N-CA-C | -6.41 | 104.71      | 113.30   |
| 13  | o     | 5208 | LEU  | N-CA-C | -6.41 | 104.71      | 113.30   |
| 2   | b     | 5331 | ASN  | N-CA-C | 6.40  | 118.33      | 111.36   |
| 13  | o     | 5086 | ARG  | N-CA-C | 6.39  | 121.89      | 113.20   |
| 2   | B     | 331  | ASN  | N-CA-C | 6.39  | 118.32      | 111.36   |
| 13  | O     | 86   | ARG  | N-CA-C | 6.38  | 121.88      | 113.20   |
| 2   | B     | 298  | LEU  | N-CA-C | -6.38 | 103.59      | 111.75   |
| 2   | b     | 5298 | LEU  | N-CA-C | -6.38 | 103.59      | 111.75   |
| 3   | C     | 134  | ILE  | N-CA-C | 6.36  | 117.46      | 112.12   |
| 2   | b     | 5305 | ILE  | CA-C-N | 6.36  | 126.86      | 119.99   |
| 2   | b     | 5305 | ILE  | C-N-CA | 6.36  | 126.86      | 119.99   |
| 3   | c     | 5134 | ILE  | N-CA-C | 6.36  | 117.46      | 112.12   |
| 15  | U     | 81   | HIS  | N-CA-C | 6.34  | 121.03      | 113.16   |
| 12  | m     | 5016 | LEU  | N-CA-C | 6.33  | 118.99      | 111.71   |
| 15  | u     | 5081 | HIS  | N-CA-C | 6.33  | 121.01      | 113.16   |
| 2   | B     | 305  | ILE  | CA-C-N | 6.33  | 126.82      | 119.99   |
| 2   | B     | 305  | ILE  | C-N-CA | 6.33  | 126.82      | 119.99   |
| 12  | M     | 16   | LEU  | N-CA-C | 6.32  | 118.98      | 111.71   |
| 15  | u     | 5040 | GLY  | N-CA-C | 6.32  | 122.71      | 113.48   |
| 15  | U     | 40   | GLY  | N-CA-C | 6.31  | 122.70      | 113.48   |
| 3   | C     | 141  | GLU  | N-CA-C | -6.31 | 104.48      | 111.36   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | c     | 5141 | GLU  | N-CA-C  | -6.30 | 104.49      | 111.36   |
| 3   | C     | 449  | ARG  | N-CA-C  | -6.30 | 105.45      | 113.01   |
| 4   | d     | 5023 | LYS  | N-CA-C  | 6.30  | 120.16      | 112.23   |
| 2   | B     | 399  | VAL  | N-CA-C  | 6.29  | 117.17      | 108.12   |
| 2   | b     | 5318 | ASN  | CA-C-N  | 6.29  | 127.70      | 119.84   |
| 2   | b     | 5318 | ASN  | C-N-CA  | 6.29  | 127.70      | 119.84   |
| 4   | D     | 23   | LYS  | N-CA-C  | 6.28  | 120.14      | 112.23   |
| 3   | c     | 5449 | ARG  | N-CA-C  | -6.28 | 105.48      | 113.01   |
| 13  | o     | 5051 | THR  | N-CA-C  | -6.27 | 104.26      | 112.41   |
| 2   | B     | 318  | ASN  | CA-C-N  | 6.27  | 127.68      | 119.84   |
| 2   | B     | 318  | ASN  | C-N-CA  | 6.27  | 127.68      | 119.84   |
| 13  | O     | 51   | THR  | N-CA-C  | -6.27 | 104.26      | 112.41   |
| 2   | b     | 5399 | VAL  | N-CA-C  | 6.26  | 117.14      | 108.12   |
| 4   | D     | 105  | CYS  | N-CA-C  | -6.26 | 105.13      | 112.89   |
| 3   | C     | 385  | GLN  | CA-C-N  | 6.25  | 125.66      | 118.85   |
| 3   | C     | 385  | GLN  | C-N-CA  | 6.25  | 125.66      | 118.85   |
| 4   | d     | 5105 | CYS  | N-CA-C  | -6.25 | 105.14      | 112.89   |
| 3   | C     | 391  | ARG  | N-CA-C  | -6.24 | 104.01      | 111.69   |
| 1   | a     | 5038 | ILE  | CA-C-N  | -6.24 | 112.04      | 119.84   |
| 1   | a     | 5038 | ILE  | C-N-CA  | -6.24 | 112.04      | 119.84   |
| 1   | A     | 38   | ILE  | CA-C-N  | -6.24 | 112.04      | 119.84   |
| 1   | A     | 38   | ILE  | C-N-CA  | -6.24 | 112.04      | 119.84   |
| 4   | d     | 5062 | GLY  | N-CA-C  | -6.24 | 104.69      | 114.10   |
| 3   | c     | 5385 | GLN  | CA-C-N  | 6.23  | 125.64      | 118.85   |
| 3   | c     | 5385 | GLN  | C-N-CA  | 6.23  | 125.64      | 118.85   |
| 3   | c     | 5391 | ARG  | N-CA-C  | -6.23 | 104.03      | 111.69   |
| 3   | C     | 88   | LEU  | N-CA-C  | 6.23  | 117.73      | 111.07   |
| 2   | B     | 487  | SER  | N-CA-C  | 6.22  | 123.57      | 109.81   |
| 2   | b     | 5487 | SER  | N-CA-C  | 6.22  | 123.57      | 109.81   |
| 4   | D     | 62   | GLY  | N-CA-C  | -6.22 | 104.70      | 114.10   |
| 11  | L     | 13   | ASN  | N-CA-C  | 6.22  | 118.94      | 110.55   |
| 11  | l     | 5013 | ASN  | N-CA-C  | 6.22  | 118.94      | 110.55   |
| 1   | A     | 341  | LEU  | N-CA-C  | 6.21  | 118.64      | 108.52   |
| 1   | a     | 5260 | PHE  | N-CA-C  | 6.21  | 124.02      | 110.80   |
| 2   | B     | 290  | ALA  | N-CA-C  | -6.21 | 104.21      | 110.97   |
| 3   | c     | 5088 | LEU  | N-CA-C  | 6.20  | 117.71      | 111.07   |
| 1   | a     | 5341 | LEU  | N-CA-C  | 6.20  | 118.63      | 108.52   |
| 14  | t     | 5021 | ILE  | CB-CA-C | -6.20 | 104.48      | 111.80   |
| 14  | T     | 21   | ILE  | CB-CA-C | -6.20 | 104.49      | 111.80   |
| 16  | v     | 5100 | ASP  | N-CA-C  | -6.20 | 103.46      | 111.02   |
| 1   | A     | 260  | PHE  | N-CA-C  | 6.20  | 124.00      | 110.80   |
| 3   | C     | 254  | THR  | N-CA-C  | 6.20  | 118.83      | 109.41   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 16  | V     | 100  | ASP  | N-CA-C  | -6.20 | 103.46      | 111.02   |
| 1   | A     | 176  | ILE  | CB-CA-C | -6.18 | 104.08      | 111.81   |
| 2   | b     | 5290 | ALA  | N-CA-C  | -6.17 | 104.24      | 110.97   |
| 1   | a     | 5176 | ILE  | CB-CA-C | -6.17 | 104.09      | 111.81   |
| 3   | c     | 5254 | THR  | N-CA-C  | 6.17  | 118.78      | 109.41   |
| 7   | H     | 48   | ILE  | N-CA-C  | -6.16 | 104.29      | 111.00   |
| 5   | e     | 5022 | ILE  | N-CA-C  | -6.13 | 104.76      | 110.53   |
| 7   | h     | 5048 | ILE  | N-CA-C  | -6.13 | 104.31      | 111.00   |
| 3   | C     | 140  | LEU  | N-CA-C  | -6.13 | 105.56      | 113.16   |
| 3   | c     | 5140 | LEU  | N-CA-C  | -6.12 | 105.56      | 113.16   |
| 5   | E     | 22   | ILE  | N-CA-C  | -6.12 | 104.78      | 110.53   |
| 3   | c     | 5043 | ILE  | N-CA-C  | -6.07 | 106.58      | 112.29   |
| 2   | B     | 14   | ASN  | N-CA-C  | -6.07 | 100.95      | 110.36   |
| 2   | b     | 5383 | PHE  | N-CA-C  | -6.06 | 105.91      | 113.55   |
| 16  | V     | 108  | TYR  | N-CA-C  | -6.05 | 105.75      | 113.02   |
| 2   | b     | 5014 | ASN  | N-CA-C  | -6.05 | 100.97      | 110.36   |
| 2   | B     | 383  | PHE  | N-CA-C  | -6.05 | 105.92      | 113.55   |
| 16  | v     | 5108 | TYR  | N-CA-C  | -6.04 | 105.77      | 113.02   |
| 3   | C     | 43   | ILE  | N-CA-C  | -6.04 | 106.61      | 112.29   |
| 1   | a     | 5312 | ASN  | N-CA-C  | -6.04 | 101.36      | 110.24   |
| 2   | b     | 5050 | PRO  | N-CA-C  | -6.03 | 106.81      | 114.35   |
| 2   | B     | 50   | PRO  | N-CA-C  | -6.03 | 106.81      | 114.35   |
| 2   | b     | 5328 | GLY  | CA-C-N  | 6.03  | 126.34      | 119.83   |
| 2   | b     | 5328 | GLY  | C-N-CA  | 6.03  | 126.34      | 119.83   |
| 14  | T     | 17   | PHE  | N-CA-C  | -6.02 | 104.08      | 112.45   |
| 3   | C     | 404  | LEU  | N-CA-C  | -6.02 | 104.05      | 111.33   |
| 16  | V     | 109  | ASP  | N-CA-C  | -6.02 | 105.60      | 113.12   |
| 1   | A     | 312  | ASN  | N-CA-C  | -6.01 | 101.40      | 110.24   |
| 1   | A     | 130  | GLN  | N-CA-C  | -6.00 | 104.67      | 112.23   |
| 14  | t     | 5017 | PHE  | N-CA-C  | -6.00 | 104.10      | 112.45   |
| 2   | B     | 328  | GLY  | CA-C-N  | 5.99  | 126.30      | 119.83   |
| 2   | B     | 328  | GLY  | C-N-CA  | 5.99  | 126.30      | 119.83   |
| 1   | a     | 5130 | GLN  | N-CA-C  | -5.99 | 104.69      | 112.23   |
| 4   | D     | 117  | HIS  | N-CA-C  | -5.98 | 104.67      | 111.07   |
| 3   | c     | 5404 | LEU  | N-CA-C  | -5.98 | 104.09      | 111.33   |
| 16  | v     | 5109 | ASP  | N-CA-C  | -5.98 | 105.64      | 113.12   |
| 13  | O     | 235  | GLY  | N-CA-C  | -5.98 | 107.07      | 115.32   |
| 7   | h     | 5025 | TRP  | N-CA-C  | -5.97 | 106.12      | 113.41   |
| 6   | f     | 5032 | PHE  | N-CA-C  | -5.97 | 104.69      | 111.14   |
| 7   | H     | 25   | TRP  | N-CA-C  | -5.97 | 106.13      | 113.41   |
| 4   | d     | 5117 | HIS  | N-CA-C  | -5.97 | 104.69      | 111.07   |
| 15  | u     | 5051 | LYS  | N-CA-C  | -5.97 | 98.09       | 110.80   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | c     | 5259 | TRP  | N-CA-C | -5.96 | 105.50      | 112.89   |
| 3   | C     | 259  | TRP  | N-CA-C | -5.96 | 105.50      | 112.89   |
| 3   | c     | 5333 | GLY  | CA-C-N | 5.96  | 127.29      | 119.84   |
| 3   | c     | 5333 | GLY  | C-N-CA | 5.96  | 127.29      | 119.84   |
| 3   | C     | 333  | GLY  | CA-C-N | 5.96  | 127.28      | 119.84   |
| 3   | C     | 333  | GLY  | C-N-CA | 5.96  | 127.28      | 119.84   |
| 3   | C     | 302  | TYR  | N-CA-C | -5.95 | 101.38      | 109.95   |
| 6   | F     | 32   | PHE  | N-CA-C | -5.95 | 104.71      | 111.14   |
| 13  | o     | 5235 | GLY  | N-CA-C | -5.95 | 107.11      | 115.32   |
| 15  | U     | 51   | LYS  | N-CA-C | -5.95 | 98.12       | 110.80   |
| 3   | c     | 5302 | TYR  | N-CA-C | -5.95 | 101.39      | 109.95   |
| 3   | C     | 229  | ASN  | N-CA-C | 5.91  | 118.21      | 109.69   |
| 3   | c     | 5229 | ASN  | N-CA-C | 5.91  | 118.19      | 109.69   |
| 5   | E     | 13   | ILE  | N-CA-C | 5.90  | 119.35      | 111.44   |
| 1   | A     | 82   | VAL  | N-CA-C | -5.88 | 99.95       | 108.36   |
| 1   | a     | 5323 | ARG  | N-CA-C | -5.88 | 104.57      | 110.97   |
| 1   | a     | 5176 | ILE  | N-CA-C | 5.87  | 116.00      | 110.30   |
| 1   | A     | 323  | ARG  | N-CA-C | -5.87 | 104.58      | 110.97   |
| 3   | C     | 466  | VAL  | N-CA-C | 5.87  | 116.64      | 110.72   |
| 1   | a     | 5082 | VAL  | N-CA-C | -5.87 | 99.97       | 108.36   |
| 5   | e     | 5013 | ILE  | N-CA-C | 5.86  | 119.30      | 111.44   |
| 3   | c     | 5466 | VAL  | N-CA-C | 5.85  | 116.63      | 110.72   |
| 16  | V     | 95   | ILE  | N-CA-C | -5.85 | 103.47      | 111.89   |
| 16  | v     | 5095 | ILE  | N-CA-C | -5.84 | 103.49      | 111.89   |
| 4   | d     | 5167 | TRP  | N-CA-C | -5.83 | 105.27      | 112.38   |
| 1   | A     | 176  | ILE  | N-CA-C | 5.82  | 115.95      | 110.30   |
| 4   | D     | 18   | LEU  | N-CA-C | -5.82 | 104.84      | 111.07   |
| 4   | d     | 5018 | LEU  | N-CA-C | -5.82 | 104.84      | 111.07   |
| 2   | b     | 5277 | SER  | N-CA-C | -5.82 | 99.81       | 109.46   |
| 1   | a     | 5263 | ALA  | N-CA-C | -5.81 | 106.42      | 112.93   |
| 15  | u     | 5049 | ILE  | N-CA-C | -5.81 | 104.66      | 110.30   |
| 2   | B     | 277  | SER  | N-CA-C | -5.81 | 99.81       | 109.46   |
| 14  | t     | 5026 | PRO  | N-CA-C | 5.81  | 117.79      | 110.70   |
| 1   | A     | 263  | ALA  | N-CA-C | -5.80 | 106.43      | 112.93   |
| 4   | D     | 167  | TRP  | N-CA-C | -5.80 | 105.30      | 112.38   |
| 15  | U     | 49   | ILE  | N-CA-C | -5.80 | 104.67      | 110.30   |
| 2   | B     | 486  | LEU  | N-CA-C | 5.80  | 116.74      | 108.74   |
| 14  | T     | 26   | PRO  | N-CA-C | 5.79  | 117.76      | 110.70   |
| 2   | b     | 5486 | LEU  | N-CA-C | 5.78  | 116.72      | 108.74   |
| 4   | D     | 259  | ILE  | N-CA-C | 5.76  | 118.25      | 108.86   |
| 1   | A     | 252  | HIS  | N-CA-C | -5.75 | 105.01      | 111.28   |
| 4   | d     | 5259 | ILE  | N-CA-C | 5.75  | 118.23      | 108.86   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 7   | H     | 55   | LEU  | N-CA-C | -5.74 | 100.63      | 108.38   |
| 12  | m     | 5028 | GLN  | N-CA-C | -5.72 | 105.02      | 112.23   |
| 12  | M     | 28   | GLN  | N-CA-C | -5.71 | 105.03      | 112.23   |
| 1   | a     | 5252 | HIS  | N-CA-C | -5.71 | 105.05      | 111.28   |
| 7   | h     | 5055 | LEU  | N-CA-C | -5.71 | 100.67      | 108.38   |
| 1   | a     | 5140 | ARG  | CA-C-N | -5.71 | 112.71      | 119.84   |
| 1   | a     | 5140 | ARG  | C-N-CA | -5.71 | 112.71      | 119.84   |
| 2   | B     | 6    | TYR  | N-CA-C | -5.70 | 105.07      | 111.28   |
| 15  | U     | 87   | VAL  | N-CA-C | -5.70 | 101.42      | 109.63   |
| 1   | A     | 140  | ARG  | CA-C-N | -5.69 | 112.73      | 119.84   |
| 1   | A     | 140  | ARG  | C-N-CA | -5.69 | 112.73      | 119.84   |
| 15  | u     | 5087 | VAL  | N-CA-C | -5.69 | 101.44      | 109.63   |
| 2   | b     | 5328 | GLY  | N-CA-C | 5.68  | 123.93      | 112.34   |
| 2   | B     | 328  | GLY  | N-CA-C | 5.68  | 123.92      | 112.34   |
| 8   | i     | 5028 | PRO  | N-CA-C | -5.68 | 106.46      | 113.84   |
| 8   | I     | 28   | PRO  | N-CA-C | -5.67 | 106.47      | 113.84   |
| 3   | c     | 5129 | GLY  | N-CA-C | -5.67 | 105.93      | 112.73   |
| 1   | a     | 5168 | PHE  | N-CA-C | -5.66 | 106.07      | 112.87   |
| 4   | D     | 25   | ASP  | N-CA-C | 5.66  | 122.86      | 110.80   |
| 1   | A     | 168  | PHE  | N-CA-C | -5.66 | 106.08      | 112.87   |
| 3   | C     | 422  | PRO  | N-CA-C | -5.65 | 105.67      | 113.53   |
| 3   | c     | 5422 | PRO  | N-CA-C | -5.65 | 105.67      | 113.53   |
| 3   | C     | 129  | GLY  | N-CA-C | -5.65 | 105.95      | 112.73   |
| 4   | d     | 5025 | ASP  | N-CA-C | 5.65  | 122.84      | 110.80   |
| 2   | b     | 5006 | TYR  | N-CA-C | -5.65 | 105.12      | 111.28   |
| 14  | T     | 25   | GLU  | CA-C-N | 5.64  | 126.19      | 120.38   |
| 14  | T     | 25   | GLU  | C-N-CA | 5.64  | 126.19      | 120.38   |
| 14  | t     | 5025 | GLU  | CA-C-N | 5.63  | 126.18      | 120.38   |
| 14  | t     | 5025 | GLU  | C-N-CA | 5.63  | 126.18      | 120.38   |
| 2   | b     | 5303 | SER  | N-CA-C | -5.62 | 106.13      | 112.87   |
| 2   | B     | 303  | SER  | N-CA-C | -5.62 | 106.13      | 112.87   |
| 3   | c     | 5272 | LEU  | N-CA-C | -5.61 | 105.09      | 111.14   |
| 1   | a     | 5313 | VAL  | N-CA-C | 5.60  | 116.64      | 108.58   |
| 3   | C     | 87   | ILE  | N-CA-C | -5.60 | 106.24      | 111.45   |
| 3   | C     | 272  | LEU  | N-CA-C | -5.60 | 105.09      | 111.14   |
| 1   | A     | 313  | VAL  | N-CA-C | 5.59  | 116.63      | 108.58   |
| 4   | D     | 228  | GLY  | N-CA-C | 5.59  | 117.20      | 111.56   |
| 2   | B     | 173  | GLY  | N-CA-C | -5.58 | 99.94       | 113.18   |
| 1   | A     | 272  | HIS  | N-CA-C | -5.58 | 104.61      | 111.75   |
| 2   | b     | 5081 | THR  | N-CA-C | -5.58 | 104.83      | 111.69   |
| 3   | c     | 5087 | ILE  | N-CA-C | -5.58 | 106.26      | 111.45   |
| 2   | b     | 5173 | GLY  | N-CA-C | -5.57 | 99.97       | 113.18   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 386  | ALA  | N-CA-C  | -5.57 | 106.65      | 113.50   |
| 2   | B     | 81   | THR  | N-CA-C  | -5.57 | 104.84      | 111.69   |
| 4   | d     | 5228 | GLY  | N-CA-C  | 5.57  | 117.19      | 111.56   |
| 7   | h     | 5009 | ASP  | N-CA-C  | -5.57 | 105.27      | 112.68   |
| 4   | D     | 344  | GLU  | N-CA-C  | 5.55  | 117.19      | 111.03   |
| 2   | b     | 5386 | ALA  | N-CA-C  | -5.55 | 106.67      | 113.50   |
| 4   | d     | 5344 | GLU  | N-CA-C  | 5.54  | 117.18      | 111.03   |
| 7   | H     | 9    | ASP  | N-CA-C  | -5.54 | 105.31      | 112.68   |
| 4   | d     | 5030 | VAL  | CA-C-N  | -5.54 | 117.24      | 122.17   |
| 4   | d     | 5030 | VAL  | C-N-CA  | -5.54 | 117.24      | 122.17   |
| 4   | D     | 30   | VAL  | CA-C-N  | -5.53 | 117.25      | 122.17   |
| 4   | D     | 30   | VAL  | C-N-CA  | -5.53 | 117.25      | 122.17   |
| 4   | d     | 5248 | THR  | N-CA-C  | -5.51 | 106.63      | 113.19   |
| 2   | b     | 5280 | PHE  | N-CA-C  | 5.51  | 118.05      | 111.71   |
| 4   | d     | 5176 | ALA  | N-CA-C  | -5.51 | 104.79      | 112.45   |
| 10  | k     | 5041 | ALA  | N-CA-C  | -5.50 | 106.24      | 113.12   |
| 4   | D     | 248  | THR  | N-CA-C  | -5.50 | 106.65      | 113.19   |
| 1   | a     | 5047 | CYS  | N-CA-C  | -5.50 | 105.19      | 111.07   |
| 4   | D     | 176  | ALA  | N-CA-C  | -5.49 | 104.82      | 112.45   |
| 4   | d     | 5179 | PHE  | N-CA-C  | -5.49 | 105.46      | 111.82   |
| 1   | A     | 47   | CYS  | N-CA-C  | -5.48 | 105.21      | 111.07   |
| 4   | D     | 179  | PHE  | N-CA-C  | -5.48 | 105.46      | 111.82   |
| 2   | B     | 54   | PRO  | N-CA-C  | -5.46 | 103.28      | 111.57   |
| 2   | b     | 5054 | PRO  | N-CA-C  | -5.45 | 103.29      | 111.57   |
| 4   | D     | 103  | ARG  | N-CA-C  | -5.45 | 105.26      | 111.14   |
| 16  | V     | 73   | LYS  | N-CA-C  | 5.44  | 117.91      | 111.33   |
| 16  | v     | 5073 | LYS  | N-CA-C  | 5.43  | 117.91      | 111.33   |
| 2   | b     | 5189 | GLY  | N-CA-C  | -5.43 | 107.10      | 115.73   |
| 2   | B     | 189  | GLY  | N-CA-C  | -5.42 | 107.11      | 115.73   |
| 4   | d     | 5103 | ARG  | N-CA-C  | -5.42 | 105.29      | 111.14   |
| 3   | C     | 258  | GLY  | N-CA-C  | 5.39  | 120.68      | 114.16   |
| 3   | c     | 5258 | GLY  | N-CA-C  | 5.39  | 120.68      | 114.16   |
| 13  | o     | 5225 | LEU  | N-CA-C  | 5.38  | 117.43      | 108.02   |
| 13  | O     | 225  | LEU  | N-CA-C  | 5.37  | 117.42      | 108.02   |
| 4   | d     | 5321 | LEU  | N-CA-C  | -5.37 | 104.67      | 111.11   |
| 4   | D     | 321  | LEU  | N-CA-C  | -5.36 | 104.68      | 111.11   |
| 20  | z     | 5002 | THR  | N-CA-C  | -5.35 | 105.49      | 112.23   |
| 2   | B     | 280  | PHE  | N-CA-C  | 5.34  | 118.02      | 111.82   |
| 2   | B     | 191  | ASN  | N-CA-C  | -5.34 | 98.01       | 109.81   |
| 20  | Z     | 2    | THR  | N-CA-C  | -5.34 | 105.50      | 112.23   |
| 2   | b     | 5008 | VAL  | CB-CA-C | -5.33 | 103.62      | 112.26   |
| 1   | a     | 5228 | THR  | N-CA-C  | -5.33 | 100.74      | 109.80   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | b     | 5363 | PHE  | N-CA-C  | 5.33  | 118.31      | 109.46   |
| 1   | A     | 228  | THR  | N-CA-C  | -5.33 | 100.74      | 109.80   |
| 2   | B     | 171  | PRO  | N-CA-C  | 5.32  | 123.44      | 112.47   |
| 2   | B     | 156  | PHE  | N-CA-C  | 5.32  | 119.49      | 112.89   |
| 2   | B     | 362  | PHE  | N-CA-C  | 5.32  | 117.99      | 111.82   |
| 2   | b     | 5191 | ASN  | N-CA-C  | -5.32 | 98.06       | 109.81   |
| 2   | b     | 5156 | PHE  | N-CA-C  | 5.32  | 119.48      | 112.89   |
| 2   | B     | 363  | PHE  | N-CA-C  | 5.31  | 118.27      | 109.46   |
| 13  | o     | 5083 | LYS  | N-CA-C  | -5.31 | 103.88      | 110.41   |
| 2   | B     | 8    | VAL  | CB-CA-C | -5.31 | 103.66      | 112.26   |
| 13  | O     | 83   | LYS  | N-CA-C  | -5.31 | 103.88      | 110.41   |
| 16  | V     | 75   | ASN  | CA-C-N  | 5.30  | 126.47      | 119.84   |
| 16  | V     | 75   | ASN  | C-N-CA  | 5.30  | 126.47      | 119.84   |
| 2   | b     | 5171 | PRO  | N-CA-C  | 5.30  | 123.38      | 112.47   |
| 3   | C     | 228  | ASN  | N-CA-C  | 5.29  | 117.46      | 111.11   |
| 2   | b     | 5362 | PHE  | N-CA-C  | 5.29  | 117.96      | 111.82   |
| 3   | c     | 5445 | ALA  | N-CA-C  | -5.28 | 105.11      | 112.45   |
| 13  | o     | 5099 | ARG  | N-CA-C  | 5.28  | 117.82      | 109.96   |
| 16  | v     | 5075 | ASN  | CA-C-N  | 5.28  | 126.44      | 119.84   |
| 16  | v     | 5075 | ASN  | C-N-CA  | 5.28  | 126.44      | 119.84   |
| 20  | Z     | 7    | LEU  | N-CA-C  | -5.28 | 105.99      | 112.90   |
| 3   | c     | 5228 | ASN  | N-CA-C  | 5.27  | 117.44      | 111.11   |
| 20  | z     | 5007 | LEU  | N-CA-C  | -5.27 | 105.99      | 112.90   |
| 13  | O     | 99   | ARG  | N-CA-C  | 5.27  | 117.81      | 109.96   |
| 5   | e     | 5079 | PHE  | N-CA-C  | -5.27 | 103.50      | 111.56   |
| 12  | M     | 5    | GLN  | N-CA-C  | 5.27  | 118.87      | 112.23   |
| 5   | E     | 79   | PHE  | N-CA-C  | -5.26 | 103.52      | 111.56   |
| 3   | C     | 135  | ARG  | N-CA-C  | 5.25  | 119.79      | 113.17   |
| 3   | C     | 445  | ALA  | N-CA-C  | -5.25 | 105.16      | 112.45   |
| 16  | v     | 5028 | GLU  | N-CA-C  | -5.24 | 106.94      | 113.55   |
| 16  | V     | 28   | GLU  | N-CA-C  | -5.24 | 106.95      | 113.55   |
| 12  | m     | 5005 | GLN  | N-CA-C  | 5.24  | 118.83      | 112.23   |
| 2   | b     | 5276 | ASP  | N-CA-C  | -5.23 | 105.27      | 110.97   |
| 2   | B     | 463  | PHE  | N-CA-C  | -5.23 | 106.00      | 112.38   |
| 3   | c     | 5135 | ARG  | N-CA-C  | 5.23  | 119.76      | 113.17   |
| 13  | O     | 151  | LEU  | N-CA-C  | 5.23  | 117.81      | 109.96   |
| 13  | o     | 5151 | LEU  | N-CA-C  | 5.23  | 117.80      | 109.96   |
| 13  | o     | 5219 | THR  | N-CA-C  | 5.23  | 117.13      | 109.24   |
| 2   | B     | 276  | ASP  | N-CA-C  | -5.22 | 105.28      | 110.97   |
| 20  | z     | 5039 | LEU  | N-CA-C  | -5.22 | 106.17      | 112.54   |
| 13  | O     | 103  | SER  | N-CA-C  | 5.22  | 117.27      | 110.43   |
| 2   | b     | 5463 | PHE  | N-CA-C  | -5.22 | 106.01      | 112.38   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 13  | o     | 5103 | SER  | N-CA-C | 5.22  | 117.27      | 110.43   |
| 1   | a     | 5065 | GLU  | N-CA-C | -5.22 | 98.00       | 109.11   |
| 20  | Z     | 39   | LEU  | N-CA-C | -5.21 | 106.18      | 112.54   |
| 4   | d     | 5282 | SER  | N-CA-C | -5.21 | 104.51      | 111.24   |
| 1   | A     | 65   | GLU  | N-CA-C | -5.21 | 98.01       | 109.11   |
| 13  | O     | 44   | LYS  | N-CA-C | -5.21 | 100.75      | 109.24   |
| 13  | o     | 5044 | LYS  | N-CA-C | -5.20 | 100.76      | 109.24   |
| 13  | O     | 219  | THR  | N-CA-C | 5.20  | 117.09      | 109.24   |
| 4   | D     | 282  | SER  | N-CA-C | -5.17 | 104.57      | 111.24   |
| 2   | b     | 5359 | MET  | CA-C-N | 5.17  | 125.33      | 119.90   |
| 2   | b     | 5359 | MET  | C-N-CA | 5.17  | 125.33      | 119.90   |
| 13  | O     | 45   | CYS  | N-CA-C | 5.16  | 118.00      | 110.10   |
| 8   | I     | 29   | ALA  | N-CA-C | -5.16 | 102.42      | 110.42   |
| 7   | H     | 27   | THR  | N-CA-C | 5.16  | 117.80      | 111.82   |
| 8   | i     | 5029 | ALA  | N-CA-C | -5.15 | 102.44      | 110.42   |
| 2   | B     | 359  | MET  | CA-C-N | 5.14  | 125.30      | 119.90   |
| 2   | B     | 359  | MET  | C-N-CA | 5.14  | 125.30      | 119.90   |
| 13  | o     | 5045 | CYS  | N-CA-C | 5.14  | 117.97      | 110.10   |
| 7   | h     | 5027 | THR  | N-CA-C | 5.14  | 117.78      | 111.82   |
| 16  | V     | 136  | LYS  | N-CA-C | -5.14 | 105.33      | 111.03   |
| 1   | A     | 311  | GLY  | N-CA-C | -5.13 | 108.25      | 114.92   |
| 4   | D     | 80   | THR  | N-CA-C | -5.13 | 98.47       | 109.81   |
| 1   | a     | 5311 | GLY  | N-CA-C | -5.13 | 108.25      | 114.92   |
| 2   | b     | 5239 | SER  | N-CA-C | -5.13 | 105.77      | 112.23   |
| 4   | d     | 5080 | THR  | N-CA-C | -5.13 | 98.47       | 109.81   |
| 2   | B     | 239  | SER  | N-CA-C | -5.13 | 105.77      | 112.23   |
| 16  | v     | 5136 | LYS  | N-CA-C | -5.12 | 105.34      | 111.03   |
| 2   | b     | 5483 | ASP  | CA-C-N | 5.10  | 126.22      | 119.84   |
| 2   | b     | 5483 | ASP  | C-N-CA | 5.10  | 126.22      | 119.84   |
| 15  | U     | 10   | VAL  | N-CA-C | 5.10  | 115.71      | 108.42   |
| 4   | d     | 5260 | ALA  | N-CA-C | 5.10  | 116.70      | 108.34   |
| 11  | l     | 5004 | ASN  | N-CA-C | -5.10 | 103.61      | 109.93   |
| 13  | O     | 60   | SER  | N-CA-C | -5.10 | 99.94       | 110.80   |
| 4   | D     | 260  | ALA  | N-CA-C | 5.09  | 116.69      | 108.34   |
| 11  | L     | 4    | ASN  | N-CA-C | -5.09 | 103.62      | 109.93   |
| 13  | o     | 5060 | SER  | N-CA-C | -5.08 | 99.97       | 110.80   |
| 15  | u     | 5010 | VAL  | N-CA-C | 5.08  | 115.68      | 108.42   |
| 3   | c     | 5203 | THR  | N-CA-C | 5.08  | 117.89      | 109.46   |
| 5   | e     | 5041 | GLY  | N-CA-C | -5.08 | 107.81      | 115.32   |
| 2   | B     | 483  | ASP  | CA-C-N | 5.07  | 126.18      | 119.84   |
| 2   | B     | 483  | ASP  | C-N-CA | 5.07  | 126.18      | 119.84   |
| 5   | E     | 41   | GLY  | N-CA-C | -5.07 | 107.81      | 115.32   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 13  | O     | 266  | TYR  | N-CA-C | -5.06 | 102.97      | 110.46   |
| 1   | A     | 259  | ILE  | N-CA-C | 5.05  | 119.86      | 109.34   |
| 3   | C     | 203  | THR  | N-CA-C | 5.05  | 117.85      | 109.46   |
| 2   | b     | 5470 | GLY  | N-CA-C | -5.04 | 106.68      | 112.73   |
| 2   | B     | 470  | GLY  | N-CA-C | -5.04 | 106.68      | 112.73   |
| 1   | a     | 5259 | ILE  | N-CA-C | 5.04  | 119.82      | 109.34   |
| 1   | A     | 265  | PHE  | N-CA-C | 5.03  | 117.17      | 109.07   |
| 13  | o     | 5266 | TYR  | N-CA-C | -5.03 | 103.02      | 110.46   |
| 1   | a     | 5265 | PHE  | N-CA-C | 5.02  | 117.15      | 109.07   |
| 4   | D     | 67   | TYR  | N-CA-C | -5.02 | 105.09      | 111.11   |

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     | 2630  | 0        | 2528     | 776     | 0            |
| 1   | a     | 2630  | 0        | 2528     | 771     | 0            |
| 2   | B     | 3835  | 0        | 3700     | 851     | 0            |
| 2   | b     | 3835  | 0        | 3700     | 836     | 0            |
| 3   | C     | 3455  | 0        | 3376     | 877     | 0            |
| 3   | c     | 3455  | 0        | 3376     | 878     | 0            |
| 4   | D     | 2706  | 0        | 2607     | 782     | 0            |
| 4   | d     | 2706  | 0        | 2608     | 777     | 0            |
| 5   | E     | 666   | 0        | 651      | 111     | 0            |
| 5   | e     | 666   | 0        | 651      | 112     | 0            |
| 6   | F     | 282   | 0        | 291      | 84      | 0            |
| 6   | f     | 282   | 0        | 291      | 83      | 0            |
| 7   | H     | 507   | 0        | 529      | 146     | 0            |
| 7   | h     | 507   | 0        | 529      | 155     | 0            |
| 8   | I     | 287   | 0        | 308      | 65      | 0            |
| 8   | i     | 287   | 0        | 305      | 64      | 0            |
| 9   | J     | 249   | 0        | 262      | 64      | 0            |
| 9   | j     | 249   | 0        | 262      | 63      | 0            |
| 10  | K     | 278   | 0        | 289      | 88      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | k     | 278   | 0        | 289      | 118     | 0            |
| 11  | L     | 304   | 0        | 316      | 82      | 0            |
| 11  | l     | 304   | 0        | 313      | 87      | 0            |
| 12  | M     | 283   | 0        | 297      | 81      | 0            |
| 12  | m     | 283   | 0        | 294      | 82      | 0            |
| 13  | O     | 1860  | 0        | 1833     | 325     | 0            |
| 13  | o     | 1860  | 0        | 1833     | 334     | 0            |
| 14  | T     | 257   | 0        | 261      | 60      | 0            |
| 14  | t     | 257   | 0        | 259      | 61      | 0            |
| 15  | U     | 783   | 0        | 779      | 143     | 0            |
| 15  | u     | 783   | 0        | 779      | 148     | 0            |
| 16  | V     | 1064  | 0        | 1072     | 218     | 0            |
| 16  | v     | 1064  | 0        | 1072     | 209     | 0            |
| 17  | X     | 246   | 0        | 269      | 39      | 0            |
| 17  | x     | 246   | 0        | 269      | 36      | 0            |
| 18  | Y     | 208   | 0        | 237      | 77      | 0            |
| 18  | y     | 208   | 0        | 237      | 76      | 0            |
| 19  | N     | 116   | 0        | 26       | 5       | 0            |
| 19  | n     | 116   | 0        | 26       | 5       | 0            |
| 20  | Z     | 479   | 0        | 516      | 74      | 0            |
| 20  | z     | 479   | 0        | 513      | 74      | 0            |
| 21  | A     | 5     | 0        | 0        | 0       | 0            |
| 21  | a     | 5     | 0        | 0        | 0       | 0            |
| 22  | A     | 195   | 0        | 216      | 133     | 0            |
| 22  | B     | 975   | 0        | 1080     | 648     | 0            |
| 22  | C     | 780   | 0        | 864      | 478     | 0            |
| 22  | D     | 195   | 0        | 216      | 151     | 0            |
| 22  | H     | 65    | 0        | 72       | 46      | 0            |
| 22  | K     | 65    | 0        | 72       | 89      | 0            |
| 22  | a     | 195   | 0        | 216      | 135     | 0            |
| 22  | b     | 975   | 0        | 1080     | 640     | 0            |
| 22  | c     | 780   | 0        | 864      | 473     | 0            |
| 22  | d     | 195   | 0        | 216      | 149     | 0            |
| 22  | h     | 65    | 0        | 72       | 47      | 0            |
| 22  | k     | 65    | 0        | 72       | 93      | 0            |
| 23  | A     | 64    | 0        | 74       | 63      | 0            |
| 23  | D     | 64    | 0        | 74       | 51      | 0            |
| 23  | a     | 64    | 0        | 74       | 63      | 0            |
| 23  | d     | 64    | 0        | 74       | 52      | 0            |
| 24  | A     | 45    | 0        | 64       | 36      | 0            |
| 24  | D     | 45    | 0        | 64       | 56      | 0            |
| 24  | a     | 45    | 0        | 64       | 35      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | d     | 45    | 0        | 64       | 55      | 0            |
| 25  | A     | 40    | 0        | 47       | 25      | 0            |
| 25  | B     | 120   | 0        | 142      | 86      | 0            |
| 25  | C     | 80    | 0        | 96       | 76      | 0            |
| 25  | D     | 40    | 0        | 48       | 40      | 0            |
| 25  | H     | 40    | 0        | 48       | 34      | 0            |
| 25  | K     | 40    | 0        | 47       | 27      | 0            |
| 25  | T     | 80    | 0        | 95       | 67      | 0            |
| 25  | Z     | 40    | 0        | 47       | 17      | 0            |
| 25  | a     | 40    | 0        | 47       | 26      | 0            |
| 25  | b     | 80    | 0        | 95       | 62      | 0            |
| 25  | c     | 40    | 0        | 48       | 36      | 0            |
| 25  | d     | 40    | 0        | 48       | 39      | 0            |
| 25  | h     | 40    | 0        | 48       | 34      | 0            |
| 25  | k     | 80    | 0        | 95       | 74      | 0            |
| 25  | t     | 40    | 0        | 48       | 44      | 0            |
| 25  | z     | 40    | 0        | 47       | 19      | 0            |
| 26  | A     | 49    | 0        | 74       | 36      | 0            |
| 26  | a     | 49    | 0        | 74       | 36      | 0            |
| 27  | A     | 1     | 0        | 0        | 1       | 0            |
| 27  | B     | 1     | 0        | 0        | 3       | 0            |
| 27  | D     | 2     | 0        | 0        | 10      | 0            |
| 27  | T     | 1     | 0        | 0        | 2       | 0            |
| 27  | a     | 1     | 0        | 0        | 0       | 0            |
| 27  | b     | 1     | 0        | 0        | 0       | 0            |
| 27  | d     | 2     | 0        | 0        | 10      | 0            |
| 27  | t     | 1     | 0        | 0        | 4       | 0            |
| 28  | B     | 48    | 0        | 72       | 39      | 0            |
| 28  | D     | 96    | 0        | 144      | 66      | 0            |
| 28  | L     | 48    | 0        | 72       | 29      | 0            |
| 28  | b     | 48    | 0        | 72       | 38      | 0            |
| 28  | d     | 96    | 0        | 144      | 67      | 0            |
| 28  | l     | 48    | 0        | 72       | 27      | 0            |
| 29  | B     | 66    | 0        | 96       | 32      | 0            |
| 29  | C     | 198   | 0        | 288      | 118     | 0            |
| 29  | b     | 66    | 0        | 96       | 34      | 0            |
| 29  | c     | 198   | 0        | 288      | 121     | 0            |
| 30  | D     | 1     | 0        | 0        | 0       | 0            |
| 30  | a     | 1     | 0        | 0        | 0       | 0            |
| 31  | F     | 43    | 0        | 30       | 17      | 0            |
| 31  | V     | 43    | 0        | 30       | 12      | 0            |
| 31  | f     | 43    | 0        | 30       | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | v     | 43    | 0        | 30       | 10      | 0            |
| All | All   | 48060 | 0        | 48531    | 11727   | 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 121.

All (11727) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5169:PHE:HB3   | 27:d:6068:IOD:I    | 1.69                     | 1.61              |
| 14:t:5012:CYS:SG   | 27:t:6066:IOD:I    | 1.65                     | 1.58              |
| 25:k:6052:BCR:H371 | 25:k:6052:BCR:C26  | 1.34                     | 1.56              |
| 22:B:1011:CLA:HED2 | 22:B:1012:CLA:CED  | 1.31                     | 1.53              |
| 22:b:6011:CLA:HED2 | 22:b:6012:CLA:CED  | 1.31                     | 1.53              |
| 25:C:1052:BCR:H371 | 25:C:1052:BCR:C26  | 1.34                     | 1.50              |
| 22:b:6016:CLA:H162 | 22:d:6008:CLA:CMA  | 1.37                     | 1.50              |
| 22:B:1016:CLA:H162 | 22:D:1008:CLA:CMA  | 1.38                     | 1.49              |
| 22:A:1003:CLA:HED2 | 22:A:1003:CLA:CAA  | 1.44                     | 1.47              |
| 22:a:6003:CLA:HED2 | 22:a:6003:CLA:CAA  | 1.43                     | 1.47              |
| 22:B:1009:CLA:CAD  | 22:B:1010:CLA:HBB2 | 1.46                     | 1.45              |
| 2:b:5065:PHE:CE2   | 22:b:6012:CLA:HMA2 | 1.53                     | 1.43              |
| 22:b:6009:CLA:CAD  | 22:b:6010:CLA:HBB2 | 1.46                     | 1.43              |
| 2:B:65:PHE:CE2     | 22:B:1012:CLA:HMA2 | 1.53                     | 1.43              |
| 22:b:6022:CLA:C14  | 22:b:6022:CLA:H93  | 1.49                     | 1.42              |
| 22:A:1003:CLA:C2   | 23:A:1038:PHO:HBB1 | 1.50                     | 1.41              |
| 22:b:6016:CLA:H52  | 22:h:6017:CLA:C9   | 1.50                     | 1.41              |
| 22:B:1009:CLA:HBA1 | 22:B:1009:CLA:CGD  | 1.49                     | 1.41              |
| 22:B:1022:CLA:H62  | 22:B:1022:CLA:C14  | 1.50                     | 1.41              |
| 22:a:6003:CLA:C2   | 23:a:6038:PHO:HBB1 | 1.50                     | 1.41              |
| 3:c:5343:ARG:NH1   | 3:c:5348:GLU:HG3   | 1.34                     | 1.41              |
| 3:C:343:ARG:NH1    | 3:C:348:GLU:HG3    | 1.34                     | 1.41              |
| 22:a:6003:CLA:H2   | 23:a:6038:PHO:CBB  | 1.52                     | 1.40              |
| 22:B:1016:CLA:H52  | 22:H:1017:CLA:C9   | 1.50                     | 1.40              |
| 22:b:6009:CLA:HBA1 | 22:b:6009:CLA:CGD  | 1.49                     | 1.40              |
| 22:b:6022:CLA:C14  | 22:b:6022:CLA:H62  | 1.49                     | 1.40              |
| 22:B:1022:CLA:C14  | 22:B:1022:CLA:H93  | 1.49                     | 1.39              |
| 22:b:6016:CLA:C16  | 22:d:6008:CLA:HMA1 | 1.52                     | 1.39              |
| 22:A:1003:CLA:H2   | 23:A:1038:PHO:CBB  | 1.52                     | 1.39              |
| 22:B:1016:CLA:C16  | 22:D:1008:CLA:HMA1 | 1.52                     | 1.38              |
| 22:b:6021:CLA:C1A  | 22:b:6021:CLA:HED2 | 1.54                     | 1.38              |
| 22:b:6009:CLA:C14  | 22:b:6009:CLA:H8   | 1.53                     | 1.38              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1023:CLA:HED2 | 22:B:1024:CLA:CBB  | 1.55                     | 1.37              |
| 22:B:1009:CLA:C14  | 22:B:1009:CLA:H8   | 1.52                     | 1.36              |
| 22:b:6016:CLA:C5   | 22:h:6017:CLA:H91  | 1.56                     | 1.36              |
| 25:c:6054:BCR:H23C | 25:c:6054:BCR:C40  | 1.52                     | 1.36              |
| 22:B:1016:CLA:C5   | 22:H:1017:CLA:H91  | 1.56                     | 1.36              |
| 22:a:6003:CLA:CED  | 22:a:6003:CLA:HAA2 | 1.56                     | 1.36              |
| 22:b:6015:CLA:HBC1 | 25:b:6045:BCR:C34  | 1.56                     | 1.36              |
| 22:c:6025:CLA:CMB  | 22:c:6025:CLA:H42  | 1.53                     | 1.36              |
| 22:C:1025:CLA:H42  | 22:C:1025:CLA:CMB  | 1.53                     | 1.35              |
| 22:d:6008:CLA:CMA  | 22:d:6008:CLA:HBA1 | 1.53                     | 1.35              |
| 22:b:6009:CLA:CED  | 22:b:6009:CLA:HAA1 | 1.54                     | 1.35              |
| 22:B:1009:CLA:CED  | 22:B:1009:CLA:HAA1 | 1.54                     | 1.35              |
| 22:B:1021:CLA:C1A  | 22:B:1021:CLA:HED2 | 1.54                     | 1.35              |
| 22:A:1003:CLA:HAA2 | 22:A:1003:CLA:CED  | 1.56                     | 1.34              |
| 22:B:1020:CLA:H161 | 22:B:1020:CLA:C10  | 1.57                     | 1.34              |
| 25:h:6049:BCR:H23C | 25:h:6049:BCR:C39  | 1.51                     | 1.34              |
| 22:B:1021:CLA:H142 | 22:B:1021:CLA:C10  | 1.57                     | 1.34              |
| 22:b:6020:CLA:C10  | 22:b:6020:CLA:H161 | 1.57                     | 1.34              |
| 25:A:1044:BCR:H371 | 25:A:1044:BCR:C39  | 1.59                     | 1.33              |
| 25:B:1048:BCR:H371 | 25:B:1048:BCR:C40  | 1.59                     | 1.33              |
| 24:D:1042:PQ9:H42  | 24:D:1042:PQ9:C39  | 1.58                     | 1.33              |
| 25:T:6048:BCR:C39  | 25:T:6048:BCR:H371 | 1.59                     | 1.33              |
| 25:T:6048:BCR:H371 | 25:T:6048:BCR:C40  | 1.59                     | 1.33              |
| 22:b:6010:CLA:H162 | 22:b:6010:CLA:C11  | 1.56                     | 1.33              |
| 22:b:6023:CLA:HED2 | 22:b:6024:CLA:CBB  | 1.55                     | 1.33              |
| 22:B:1009:CLA:C2A  | 22:B:1009:CLA:HED3 | 1.58                     | 1.32              |
| 22:B:1015:CLA:HBC1 | 25:B:1045:BCR:C34  | 1.55                     | 1.32              |
| 22:b:6009:CLA:HED3 | 22:b:6009:CLA:C2A  | 1.58                     | 1.32              |
| 22:d:6005:CLA:HAA2 | 24:d:6042:PQ9:C41  | 1.59                     | 1.32              |
| 25:A:1044:BCR:H371 | 25:A:1044:BCR:C40  | 1.59                     | 1.32              |
| 22:c:6032:CLA:HAB  | 22:k:6034:CLA:CMC  | 1.57                     | 1.32              |
| 22:C:1032:CLA:HAB  | 22:K:1034:CLA:CMC  | 1.57                     | 1.32              |
| 24:D:1042:PQ9:H391 | 24:D:1042:PQ9:C42  | 1.49                     | 1.32              |
| 25:a:6044:BCR:H371 | 25:a:6044:BCR:C40  | 1.59                     | 1.31              |
| 22:D:1005:CLA:HAA2 | 24:D:1042:PQ9:C41  | 1.59                     | 1.31              |
| 22:D:1008:CLA:CMA  | 22:D:1008:CLA:HBA1 | 1.53                     | 1.31              |
| 25:H:1049:BCR:H23C | 25:H:1049:BCR:C39  | 1.51                     | 1.31              |
| 22:B:1010:CLA:H162 | 22:B:1010:CLA:C11  | 1.56                     | 1.31              |
| 25:a:6044:BCR:H371 | 25:a:6044:BCR:C39  | 1.59                     | 1.31              |
| 23:d:6039:PHO:HBA2 | 23:d:6039:PHO:CMA  | 1.51                     | 1.31              |
| 22:B:1011:CLA:CED  | 22:B:1012:CLA:HED1 | 1.61                     | 1.30              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B:1047:BCR:H371 | 25:B:1047:BCR:C39  | 1.59                     | 1.30              |
| 28:b:6060:MGE:H212 | 28:b:6060:MGE:CFB  | 1.54                     | 1.30              |
| 25:b:6047:BCR:H371 | 25:b:6047:BCR:C40  | 1.59                     | 1.30              |
| 25:B:1048:BCR:H371 | 25:B:1048:BCR:C39  | 1.59                     | 1.30              |
| 25:B:1047:BCR:H371 | 25:B:1047:BCR:C40  | 1.59                     | 1.30              |
| 3:C:50:LEU:C       | 3:C:50:LEU:HD23    | 1.57                     | 1.30              |
| 25:C:1052:BCR:H371 | 25:C:1052:BCR:C38  | 1.61                     | 1.30              |
| 25:b:6047:BCR:H371 | 25:b:6047:BCR:C39  | 1.59                     | 1.29              |
| 4:D:160:TYR:OH     | 27:D:1068:IOD:I    | 2.20                     | 1.29              |
| 4:d:5169:PHE:O     | 27:d:6068:IOD:I    | 2.20                     | 1.29              |
| 28:d:6059:MGE:CBB  | 28:d:6059:MGE:H251 | 1.60                     | 1.29              |
| 25:k:6052:BCR:H371 | 25:k:6052:BCR:C38  | 1.61                     | 1.28              |
| 22:b:6011:CLA:CED  | 22:b:6012:CLA:HED1 | 1.61                     | 1.28              |
| 22:C:1027:CLA:H171 | 22:C:1027:CLA:C12  | 1.59                     | 1.28              |
| 22:b:6023:CLA:H13  | 22:b:6024:CLA:CMA  | 1.64                     | 1.28              |
| 25:C:1054:BCR:H23C | 25:C:1054:BCR:C40  | 1.52                     | 1.27              |
| 25:A:1044:BCR:H392 | 25:A:1044:BCR:C37  | 1.65                     | 1.27              |
| 22:C:1032:CLA:H151 | 10:K:33:PHE:CZ     | 1.67                     | 1.27              |
| 25:b:6047:BCR:H371 | 25:b:6047:BCR:C30  | 1.65                     | 1.27              |
| 2:b:5475:PHE:CE1   | 4:d:5140:PRO:HG3   | 1.68                     | 1.26              |
| 3:c:5050:LEU:HD23  | 3:c:5050:LEU:C     | 1.57                     | 1.26              |
| 22:c:6029:CLA:H42  | 22:c:6029:CLA:C4C  | 1.63                     | 1.26              |
| 2:B:475:PHE:CE1    | 4:D:140:PRO:HG3    | 1.68                     | 1.26              |
| 24:d:6042:PQ9:H42  | 24:d:6042:PQ9:C39  | 1.58                     | 1.26              |
| 23:D:1039:PHO:HBA2 | 23:D:1039:PHO:CMA  | 1.51                     | 1.26              |
| 25:a:6044:BCR:H371 | 25:a:6044:BCR:C30  | 1.65                     | 1.26              |
| 25:a:6044:BCR:C37  | 25:a:6044:BCR:H392 | 1.65                     | 1.26              |
| 22:b:6021:CLA:H142 | 22:b:6021:CLA:C10  | 1.57                     | 1.26              |
| 22:c:6027:CLA:C12  | 22:c:6027:CLA:H171 | 1.59                     | 1.26              |
| 22:C:1025:CLA:H12  | 22:C:1025:CLA:CHB  | 1.66                     | 1.26              |
| 22:C:1029:CLA:H42  | 22:C:1029:CLA:C4C  | 1.62                     | 1.26              |
| 16:V:64:ALA:O      | 16:V:68:VAL:HG12   | 1.35                     | 1.25              |
| 22:b:6022:CLA:C9   | 22:b:6022:CLA:HBC3 | 1.66                     | 1.25              |
| 24:d:6042:PQ9:H391 | 24:d:6042:PQ9:C42  | 1.49                     | 1.25              |
| 25:A:1044:BCR:C37  | 25:A:1044:BCR:H403 | 1.65                     | 1.25              |
| 25:B:1048:BCR:H392 | 25:B:1048:BCR:C37  | 1.66                     | 1.25              |
| 22:d:6008:CLA:H193 | 22:d:6008:CLA:C14  | 1.65                     | 1.25              |
| 25:A:1044:BCR:H371 | 25:A:1044:BCR:C30  | 1.65                     | 1.25              |
| 22:B:1023:CLA:H13  | 22:B:1024:CLA:CMA  | 1.64                     | 1.25              |
| 25:B:1047:BCR:H371 | 25:B:1047:BCR:C30  | 1.65                     | 1.25              |
| 25:B:1048:BCR:C37  | 25:B:1048:BCR:H403 | 1.66                     | 1.25              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:D:1008:CLA:H193 | 22:D:1008:CLA:C14  | 1.65                     | 1.25              |
| 28:D:1059:MGE:H251 | 28:D:1059:MGE:CBB  | 1.60                     | 1.25              |
| 22:B:1009:CLA:HBD  | 22:B:1010:CLA:CBB  | 1.65                     | 1.25              |
| 25:B:1047:BCR:H392 | 25:B:1047:BCR:C37  | 1.66                     | 1.25              |
| 25:T:6048:BCR:H371 | 25:T:6048:BCR:C30  | 1.65                     | 1.25              |
| 29:b:6058:DGD:HBF2 | 29:b:6058:DGD:CIB  | 1.65                     | 1.25              |
| 22:c:6025:CLA:H12  | 22:c:6025:CLA:CHB  | 1.66                     | 1.25              |
| 22:B:1022:CLA:HBC3 | 22:B:1022:CLA:C9   | 1.65                     | 1.24              |
| 29:B:1058:DGD:HBF2 | 29:B:1058:DGD:CIB  | 1.65                     | 1.24              |
| 22:D:1005:CLA:CAA  | 24:D:1042:PQ9:H412 | 1.66                     | 1.24              |
| 25:a:6044:BCR:C37  | 25:a:6044:BCR:H403 | 1.65                     | 1.24              |
| 25:b:6047:BCR:C37  | 25:b:6047:BCR:H392 | 1.66                     | 1.24              |
| 25:T:6048:BCR:H392 | 25:T:6048:BCR:C37  | 1.66                     | 1.24              |
| 22:b:6009:CLA:HBD  | 22:b:6010:CLA:CBB  | 1.65                     | 1.24              |
| 22:B:1022:CLA:C9   | 22:B:1022:CLA:H122 | 1.67                     | 1.24              |
| 22:K:1034:CLA:HAA2 | 22:K:1034:CLA:O1D  | 1.35                     | 1.24              |
| 22:b:6022:CLA:C9   | 22:b:6022:CLA:H122 | 1.67                     | 1.24              |
| 25:b:6047:BCR:C37  | 25:b:6047:BCR:H403 | 1.66                     | 1.24              |
| 22:C:1030:CLA:H172 | 22:C:1030:CLA:C12  | 1.64                     | 1.24              |
| 22:d:6005:CLA:CAA  | 24:d:6042:PQ9:H412 | 1.66                     | 1.23              |
| 25:T:6048:BCR:C37  | 25:T:6048:BCR:H403 | 1.66                     | 1.23              |
| 25:B:1048:BCR:H371 | 25:B:1048:BCR:C30  | 1.65                     | 1.23              |
| 28:B:1060:MGE:H212 | 28:B:1060:MGE:CFB  | 1.54                     | 1.23              |
| 3:c:5265:ILE:CD1   | 3:c:5452:ALA:HB2   | 1.68                     | 1.23              |
| 22:k:6034:CLA:HAA2 | 22:k:6034:CLA:O1D  | 1.35                     | 1.23              |
| 26:a:6063:LHG:H341 | 26:a:6063:LHG:C38  | 1.65                     | 1.22              |
| 22:B:1022:CLA:HAA1 | 22:B:1022:CLA:CGD  | 1.70                     | 1.22              |
| 25:B:1047:BCR:C37  | 25:B:1047:BCR:H403 | 1.66                     | 1.22              |
| 3:C:265:ILE:CD1    | 3:C:452:ALA:HB2    | 1.68                     | 1.22              |
| 16:v:5064:ALA:O    | 16:v:5068:VAL:HG12 | 1.35                     | 1.22              |
| 22:b:6011:CLA:H3A  | 22:b:6011:CLA:CGA  | 1.60                     | 1.21              |
| 22:D:1008:CLA:H143 | 22:D:1008:CLA:C19  | 1.70                     | 1.21              |
| 22:B:1020:CLA:H161 | 22:B:1020:CLA:H102 | 1.23                     | 1.20              |
| 10:k:5032:PHE:HE1  | 25:k:6052:BCR:C22  | 1.52                     | 1.20              |
| 1:A:279:ARG:NH1    | 23:A:1038:PHO:HMC2 | 1.54                     | 1.20              |
| 22:B:1021:CLA:HED3 | 22:B:1021:CLA:C2A  | 1.72                     | 1.20              |
| 22:b:6009:CLA:CBD  | 22:b:6010:CLA:CBB  | 2.20                     | 1.20              |
| 22:b:6022:CLA:HAA1 | 22:b:6022:CLA:CGD  | 1.70                     | 1.20              |
| 26:A:1063:LHG:H341 | 26:A:1063:LHG:C38  | 1.64                     | 1.20              |
| 4:D:253:TRP:HA     | 4:D:256:ILE:HG22   | 1.23                     | 1.20              |
| 2:B:172:TYR:O      | 2:B:174:LEU:HA     | 1.41                     | 1.20              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1009:CLA:HED3 | 22:B:1009:CLA:CAA  | 1.72                     | 1.20              |
| 22:b:6021:CLA:C2A  | 22:b:6021:CLA:HED3 | 1.72                     | 1.20              |
| 22:b:6011:CLA:H12  | 22:b:6013:CLA:H93  | 1.24                     | 1.19              |
| 22:c:6025:CLA:OBD  | 22:c:6025:CLA:HED3 | 1.40                     | 1.19              |
| 22:A:1003:CLA:C4   | 22:A:1003:CLA:H71  | 1.68                     | 1.19              |
| 22:B:1011:CLA:C19  | 22:H:1017:CLA:H101 | 1.72                     | 1.19              |
| 22:d:6008:CLA:H143 | 22:d:6008:CLA:C19  | 1.70                     | 1.19              |
| 28:B:1060:MGE:H251 | 28:B:1060:MGE:CBB  | 1.72                     | 1.19              |
| 29:c:6057:DGD:CIB  | 29:c:6057:DGD:HBFB | 1.73                     | 1.19              |
| 22:C:1025:CLA:HED3 | 22:C:1025:CLA:OBD  | 1.40                     | 1.19              |
| 22:b:6009:CLA:HED3 | 22:b:6009:CLA:CAA  | 1.72                     | 1.19              |
| 4:d:5169:PHE:CB    | 27:d:6068:IOD:I    | 2.61                     | 1.19              |
| 2:b:5172:TYR:O     | 2:b:5174:LEU:HA    | 1.41                     | 1.19              |
| 22:c:6037:CLA:HBC2 | 22:c:6037:CLA:HHD  | 1.25                     | 1.19              |
| 22:B:1009:CLA:CBF  | 22:B:1010:CLA:CBB  | 2.20                     | 1.18              |
| 29:C:1056:DGD:HBFB | 29:C:1056:DGD:CIB  | 1.70                     | 1.18              |
| 1:A:279:ARG:HH11   | 23:A:1038:PHO:CMC  | 1.54                     | 1.18              |
| 22:B:1016:CLA:H2   | 22:H:1017:CLA:H93  | 1.20                     | 1.18              |
| 22:b:6011:CLA:C19  | 22:h:6017:CLA:H101 | 1.72                     | 1.18              |
| 22:c:6030:CLA:H172 | 22:c:6030:CLA:C12  | 1.64                     | 1.18              |
| 22:B:1011:CLA:H12  | 22:B:1013:CLA:H93  | 1.24                     | 1.18              |
| 23:a:6038:PHO:H201 | 22:d:6005:CLA:C2B  | 1.73                     | 1.18              |
| 29:c:6056:DGD:HBG2 | 29:c:6056:DGD:CEB  | 1.71                     | 1.18              |
| 22:B:1009:CLA:H121 | 22:B:1009:CLA:C9   | 1.73                     | 1.17              |
| 29:C:1057:DGD:HBFB | 29:C:1057:DGD:CIB  | 1.73                     | 1.17              |
| 1:a:5205:VAL:HA    | 1:a:5279:ARG:HH11  | 1.04                     | 1.17              |
| 22:a:6003:CLA:HED2 | 22:a:6003:CLA:C2A  | 1.72                     | 1.17              |
| 22:b:6018:CLA:C10  | 22:b:6023:CLA:HAA1 | 1.74                     | 1.17              |
| 22:c:6025:CLA:C15  | 22:c:6031:CLA:H92  | 1.74                     | 1.17              |
| 22:c:6030:CLA:H121 | 22:c:6030:CLA:C17  | 1.74                     | 1.17              |
| 23:A:1038:PHO:H201 | 22:D:1005:CLA:C2B  | 1.73                     | 1.17              |
| 22:B:1011:CLA:CGA  | 22:B:1011:CLA:H3A  | 1.60                     | 1.17              |
| 22:B:1018:CLA:C10  | 22:B:1023:CLA:HAA1 | 1.74                     | 1.17              |
| 3:C:46:SER:HB2     | 3:C:141:GLU:HB2    | 1.21                     | 1.17              |
| 29:C:1056:DGD:HD61 | 29:C:1056:DGD:C3E  | 1.73                     | 1.17              |
| 25:T:6046:BCR:H281 | 22:b:6015:CLA:HAC2 | 1.25                     | 1.17              |
| 22:b:6022:CLA:HAA1 | 22:b:6022:CLA:O1D  | 1.45                     | 1.17              |
| 4:d:5201:VAL:HG23  | 22:d:6004:CLA:HMB2 | 1.27                     | 1.17              |
| 22-K:1034:CLA:HAA2 | 22-K:1034:CLA:CGD  | 1.76                     | 1.16              |
| 22:c:6029:CLA:H51  | 22:c:6029:CLA:C4B  | 1.75                     | 1.16              |
| 29:c:6056:DGD:HBFB | 29:c:6056:DGD:CIB  | 1.70                     | 1.16              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:k:6051:BCR:H23C | 25:k:6051:BCR:H403 | 1.22                     | 1.16              |
| 22:B:1015:CLA:HAC2 | 25:t:1046:BCR:H281 | 1.25                     | 1.16              |
| 2:b:5169:SER:HB3   | 2:b:5176:GLY:HA2   | 1.24                     | 1.16              |
| 31:f:6040:HEM:HBA2 | 31:f:6040:HEM:CMA  | 1.68                     | 1.16              |
| 31:F:1040:HEM:HBA2 | 31:F:1040:HEM:CMA  | 1.68                     | 1.16              |
| 22:a:6003:CLA:C4   | 22:a:6003:CLA:H71  | 1.68                     | 1.16              |
| 22:c:6035:CLA:H8   | 25:k:6052:BCR:C40  | 1.76                     | 1.16              |
| 22:A:1003:CLA:HED2 | 22:A:1003:CLA:C2A  | 1.72                     | 1.16              |
| 28:b:6060:MGE:H251 | 28:b:6060:MGE:CBB  | 1.72                     | 1.16              |
| 22:A:1003:CLA:C14  | 23:A:1038:PHO:H8   | 1.76                     | 1.16              |
| 22:B:1009:CLA:H91  | 22:B:1009:CLA:C12  | 1.72                     | 1.16              |
| 22:c:6035:CLA:H8   | 25:k:6052:BCR:H403 | 1.19                     | 1.16              |
| 22:k:6034:CLA:C4   | 22:k:6034:CLA:H71  | 1.70                     | 1.16              |
| 1:A:279:ARG:HD3    | 4:D:208:ALA:HB1    | 1.22                     | 1.15              |
| 2:B:169:SER:HB3    | 2:B:176:GLY:HA2    | 1.24                     | 1.15              |
| 22:B:1010:CLA:H112 | 22:B:1010:CLA:C16  | 1.71                     | 1.15              |
| 29:C:1056:DGD:HBG2 | 29:C:1056:DGD:CEB  | 1.71                     | 1.15              |
| 2:b:5475:PHE:CD1   | 4:d:5140:PRO:HG3   | 1.82                     | 1.15              |
| 22:b:6011:CLA:H3A  | 22:b:6011:CLA:O1A  | 1.43                     | 1.15              |
| 22:B:1021:CLA:H2A  | 22:B:1021:CLA:CED  | 1.76                     | 1.15              |
| 29:C:1057:DGD:C8B  | 28:D:1059:MGE:H8B2 | 1.75                     | 1.15              |
| 4:D:139:ARG:HH12   | 4:D:265:ARG:NH2    | 1.43                     | 1.15              |
| 25:T:6046:BCR:H401 | 2:b:5036:SER:HB3   | 1.27                     | 1.15              |
| 29:c:6057:DGD:C8B  | 28:d:6059:MGE:H8B2 | 1.75                     | 1.15              |
| 4:d:5139:ARG:HH12  | 4:d:5265:ARG:NH2   | 1.43                     | 1.15              |
| 22:d:6005:CLA:CBC  | 22:d:6004:CLA:HBB2 | 1.77                     | 1.15              |
| 22:k:6034:CLA:HAA2 | 22:k:6034:CLA:CGD  | 1.75                     | 1.15              |
| 22:A:1006:CLA:HBC3 | 22:A:1006:CLA:HHD  | 1.24                     | 1.15              |
| 22:B:1016:CLA:H193 | 22:H:1017:CLA:H191 | 1.21                     | 1.15              |
| 22:C:1029:CLA:C4B  | 22:C:1029:CLA:H51  | 1.75                     | 1.15              |
| 22:K:1034:CLA:C4   | 22:K:1034:CLA:H71  | 1.70                     | 1.15              |
| 22:b:6016:CLA:H193 | 22:h:6017:CLA:H191 | 1.21                     | 1.15              |
| 4:d:5253:TRP:HA    | 4:d:5256:ILE:HG22  | 1.23                     | 1.15              |
| 2:B:174:LEU:HD23   | 2:B:266:GLU:HG2    | 1.28                     | 1.15              |
| 22:C:1025:CLA:C15  | 22:C:1031:CLA:H92  | 1.74                     | 1.15              |
| 22:C:1030:CLA:C17  | 22:C:1030:CLA:H121 | 1.74                     | 1.15              |
| 22:C:1035:CLA:H8   | 25:C:1052:BCR:H403 | 1.19                     | 1.15              |
| 26:a:6063:LHG:H383 | 26:a:6063:LHG:C34  | 1.72                     | 1.15              |
| 22:b:6016:CLA:H2   | 22:h:6017:CLA:H93  | 1.20                     | 1.15              |
| 1:A:321:ILE:HD11   | 4:D:176:ALA:HB1    | 1.25                     | 1.14              |
| 22:B:1015:CLA:C7   | 22:B:1015:CLA:H41  | 1.76                     | 1.14              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1031:CLA:HBC2 | 22:C:1031:CLA:HHD  | 1.24                     | 1.14              |
| 22:C:1035:CLA:H8   | 25:C:1052:BCR:C40  | 1.76                     | 1.14              |
| 25:D:1050:BCR:C37  | 28:D:1059:MGE:H3A1 | 1.78                     | 1.14              |
| 22:b:6009:CLA:CAD  | 22:b:6010:CLA:CBB  | 2.25                     | 1.14              |
| 22:b:6015:CLA:OBD  | 22:b:6015:CLA:HED2 | 1.46                     | 1.14              |
| 22:B:1022:CLA:HAA1 | 22:B:1022:CLA:O1D  | 1.45                     | 1.14              |
| 2:b:5174:LEU:HD22  | 2:b:5312:TYR:OH    | 1.48                     | 1.14              |
| 22:b:6015:CLA:HBC1 | 25:b:6045:BCR:H342 | 1.27                     | 1.14              |
| 22:b:6015:CLA:HBC1 | 25:b:6045:BCR:H343 | 1.28                     | 1.14              |
| 22:A:1007:CLA:OBD  | 22:A:1007:CLA:HED2 | 1.48                     | 1.14              |
| 2:B:149:LEU:HG     | 22:B:1011:CLA:HBC1 | 1.24                     | 1.14              |
| 22:B:1009:CLA:CAD  | 22:B:1010:CLA:CBB  | 2.25                     | 1.14              |
| 22:B:1014:CLA:HBC2 | 22:B:1014:CLA:HHD  | 1.24                     | 1.14              |
| 25:Z:1053:BCR:H372 | 25:Z:1053:BCR:H361 | 1.19                     | 1.14              |
| 22:b:6014:CLA:H41  | 22:b:6014:CLA:C7   | 1.75                     | 1.14              |
| 25:d:6050:BCR:C37  | 28:d:6059:MGE:H3A1 | 1.78                     | 1.14              |
| 26:A:1063:LHG:H383 | 26:A:1063:LHG:C34  | 1.71                     | 1.14              |
| 2:B:475:PHE:CD1    | 4:D:140:PRO:HG3    | 1.81                     | 1.14              |
| 22:D:1005:CLA:CBC  | 22:D:1004:CLA:HBB2 | 1.77                     | 1.14              |
| 1:a:5321:ILE:HD11  | 4:d:5176:ALA:HB1   | 1.25                     | 1.14              |
| 22:C:1025:CLA:H141 | 22:C:1031:CLA:HMB3 | 1.20                     | 1.14              |
| 1:a:5205:VAL:CB    | 1:a:5279:ARG:HH12  | 1.60                     | 1.14              |
| 29:b:6058:DGD:HBT1 | 29:b:6058:DGD:HB61 | 1.20                     | 1.14              |
| 2:B:65:PHE:CE2     | 22:B:1012:CLA:CMA  | 2.31                     | 1.13              |
| 22:C:1032:CLA:HAB  | 22:K:1034:CLA:HMC3 | 1.17                     | 1.13              |
| 10:k:5032:PHE:CE1  | 25:k:6052:BCR:C22  | 2.30                     | 1.13              |
| 22:A:1006:CLA:H172 | 25:D:1050:BCR:H282 | 1.29                     | 1.13              |
| 22:b:6009:CLA:CMB  | 25:h:6049:BCR:H271 | 1.77                     | 1.13              |
| 22:b:6021:CLA:H2A  | 22:b:6021:CLA:CED  | 1.76                     | 1.13              |
| 22:c:6025:CLA:H141 | 22:c:6031:CLA:HMB3 | 1.20                     | 1.13              |
| 6:f:5045:ARG:HA    | 6:f:5045:ARG:HE    | 1.13                     | 1.13              |
| 22:k:6034:CLA:H43  | 22:k:6034:CLA:CGA  | 1.77                     | 1.13              |
| 22:C:1025:CLA:H12  | 22:C:1025:CLA:HHB  | 1.22                     | 1.13              |
| 22:C:1031:CLA:OBD  | 22:C:1033:CLA:H122 | 1.47                     | 1.13              |
| 22:K:1034:CLA:CGA  | 22:K:1034:CLA:H43  | 1.77                     | 1.13              |
| 22:a:6003:CLA:C14  | 23:a:6038:PHO:H8   | 1.76                     | 1.13              |
| 22:a:6007:CLA:OBD  | 22:a:6007:CLA:HED2 | 1.48                     | 1.13              |
| 22:B:1011:CLA:H3A  | 22:B:1011:CLA:O1A  | 1.43                     | 1.13              |
| 22:B:1015:CLA:OBD  | 22:B:1015:CLA:HED2 | 1.46                     | 1.13              |
| 1:A:258:LEU:HD12   | 4:D:128:ARG:HH21   | 1.14                     | 1.12              |
| 2:B:36:SER:HB3     | 25:t:1046:BCR:H401 | 1.27                     | 1.12              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1009:CLA:CMB  | 25:H:1049:BCR:H271 | 1.77                     | 1.12              |
| 22:B:1022:CLA:H11  | 22:B:1022:CLA:C4D  | 1.79                     | 1.12              |
| 25:B:1045:BCR:H23C | 25:B:1045:BCR:H383 | 1.30                     | 1.13              |
| 29:B:1058:DGD:CEB  | 29:B:1058:DGD:HGB2 | 1.74                     | 1.12              |
| 22:b:6009:CLA:H121 | 22:b:6009:CLA:C9   | 1.73                     | 1.13              |
| 22:b:6018:CLA:HHC  | 22:b:6018:CLA:HBB1 | 1.31                     | 1.13              |
| 22:b:6022:CLA:H11  | 22:b:6022:CLA:C4D  | 1.79                     | 1.13              |
| 22:c:6037:CLA:HBB1 | 22:c:6037:CLA:HHC  | 1.31                     | 1.12              |
| 22:C:1037:CLA:HHD  | 22:C:1037:CLA:HBC2 | 1.25                     | 1.12              |
| 6:F:45:ARG:HA      | 6:F:45:ARG:HE      | 1.13                     | 1.12              |
| 2:b:5065:PHE:CE2   | 22:b:6012:CLA:CMA  | 2.31                     | 1.12              |
| 25:b:6045:BCR:H23C | 25:b:6045:BCR:H383 | 1.30                     | 1.12              |
| 29:b:6058:DGD:HGB2 | 29:b:6058:DGD:CEB  | 1.74                     | 1.12              |
| 3:c:5046:SER:CB    | 3:c:5141:GLU:HB2   | 1.80                     | 1.12              |
| 22:c:6035:CLA:HHC  | 22:c:6035:CLA:HBB1 | 1.30                     | 1.12              |
| 1:A:337:HIS:O      | 4:D:351:ALA:HB2    | 1.50                     | 1.12              |
| 2:b:5149:LEU:HG    | 22:b:6011:CLA:HBC1 | 1.24                     | 1.12              |
| 28:d:6059:MGE:H251 | 28:d:6059:MGE:H211 | 1.15                     | 1.12              |
| 22:b:6011:CLA:C2D  | 22:b:6013:CLA:H42  | 1.79                     | 1.12              |
| 22:b:6023:CLA:H13  | 22:b:6024:CLA:HMA3 | 1.17                     | 1.12              |
| 22:c:6031:CLA:OBD  | 22:c:6033:CLA:H122 | 1.47                     | 1.12              |
| 10:k:5032:PHE:HZ   | 25:k:6052:BCR:H361 | 1.11                     | 1.12              |
| 22:B:1022:CLA:HHD  | 22:B:1022:CLA:HBC2 | 1.26                     | 1.11              |
| 4:D:88:SER:HA      | 7:H:50:ASN:HD21    | 1.12                     | 1.11              |
| 10:k:5039:VAL:HG22 | 18:y:5036:ILE:HD11 | 1.27                     | 1.11              |
| 3:C:49:LEU:HD22    | 3:C:52:ALA:H       | 1.01                     | 1.11              |
| 3:C:275:SER:HB3    | 22:C:1033:CLA:CED  | 1.79                     | 1.11              |
| 22:a:6003:CLA:H71  | 22:a:6003:CLA:H41  | 1.31                     | 1.11              |
| 3:c:5275:SER:HB3   | 22:c:6033:CLA:CED  | 1.79                     | 1.11              |
| 22:c:6031:CLA:HHD  | 22:c:6031:CLA:HBC2 | 1.24                     | 1.11              |
| 2:b:5174:LEU:HD23  | 2:b:5266:GLU:HG2   | 1.28                     | 1.11              |
| 22:B:1011:CLA:C2D  | 22:B:1013:CLA:H42  | 1.79                     | 1.11              |
| 25:K:1051:BCR:H403 | 25:K:1051:BCR:H23C | 1.22                     | 1.11              |
| 22:b:6015:CLA:HED2 | 22:b:6015:CLA:CAD  | 1.79                     | 1.11              |
| 3:c:5049:LEU:HD21  | 22:c:6035:CLA:HMA3 | 1.25                     | 1.11              |
| 25:k:6051:BCR:H353 | 18:y:5032:GLY:HA3  | 1.32                     | 1.11              |
| 22:A:1003:CLA:H142 | 23:A:1038:PHO:H8   | 1.17                     | 1.11              |
| 22:B:1015:CLA:HED2 | 22:B:1015:CLA:CAD  | 1.79                     | 1.11              |
| 3:C:46:SER:CB      | 3:C:141:GLU:HB2    | 1.80                     | 1.11              |
| 22:C:1025:CLA:H151 | 22:C:1031:CLA:C9   | 1.80                     | 1.11              |
| 22:C:1026:CLA:H71  | 22:C:1026:CLA:H122 | 1.33                     | 1.11              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:D:1042:PQ9:H301 | 24:D:1042:PQ9:H342 | 1.32                     | 1.11              |
| 22:b:6020:CLA:HED1 | 22:b:6021:CLA:HMB2 | 1.32                     | 1.11              |
| 22:c:6030:CLA:HHD  | 22:c:6030:CLA:HBC2 | 1.32                     | 1.11              |
| 24:d:6042:PQ9:H342 | 24:d:6042:PQ9:H301 | 1.32                     | 1.11              |
| 25:d:6050:BCR:H372 | 28:d:6059:MGE:H3A1 | 1.16                     | 1.11              |
| 22:A:1006:CLA:H172 | 25:D:1050:BCR:C28  | 1.80                     | 1.10              |
| 22:b:6009:CLA:H91  | 22:b:6009:CLA:C12  | 1.72                     | 1.10              |
| 4:d:5088:SER:HA    | 7:h:5050:ASN:HD21  | 1.12                     | 1.10              |
| 26:A:1063:LHG:H291 | 22:C:1032:CLA:C7   | 1.81                     | 1.10              |
| 2:B:5:TRP:HA       | 2:B:8:VAL:HG13     | 1.34                     | 1.10              |
| 22:B:1015:CLA:HBC1 | 25:B:1045:BCR:H342 | 1.27                     | 1.10              |
| 29:B:1058:DGD:HBT1 | 29:B:1058:DGD:HB61 | 1.20                     | 1.10              |
| 22:C:1032:CLA:C15  | 10:K:33:PHE:HZ     | 1.65                     | 1.10              |
| 25:D:1050:BCR:H23C | 25:D:1050:BCR:H383 | 1.11                     | 1.10              |
| 22:b:6016:CLA:H2   | 22:h:6017:CLA:C9   | 1.81                     | 1.10              |
| 29:c:6056:DGD:HD61 | 29:c:6056:DGD:C3E  | 1.73                     | 1.10              |
| 22:B:1011:CLA:CMD  | 22:B:1013:CLA:H42  | 1.82                     | 1.10              |
| 22:b:6014:CLA:HHD  | 22:b:6014:CLA:HBC2 | 1.24                     | 1.10              |
| 22:b:6022:CLA:HBC2 | 22:b:6022:CLA:HHD  | 1.26                     | 1.10              |
| 3:c:5046:SER:HB2   | 3:c:5141:GLU:HB2   | 1.21                     | 1.10              |
| 22:B:1014:CLA:C7   | 22:B:1014:CLA:H41  | 1.75                     | 1.10              |
| 22:B:1015:CLA:HBC1 | 25:B:1045:BCR:H343 | 1.28                     | 1.10              |
| 22:B:1022:CLA:C9   | 22:B:1022:CLA:H142 | 1.82                     | 1.10              |
| 22:b:6020:CLA:H161 | 22:b:6020:CLA:H102 | 1.23                     | 1.10              |
| 3:c:5049:LEU:HD22  | 3:c:5052:ALA:H     | 1.01                     | 1.10              |
| 22:c:6032:CLA:HAB  | 22:k:6034:CLA:HMC3 | 1.17                     | 1.10              |
| 25:z:6053:BCR:H361 | 25:z:6053:BCR:H372 | 1.19                     | 1.10              |
| 22:A:1003:CLA:H71  | 22:A:1003:CLA:H41  | 1.31                     | 1.10              |
| 22:C:1030:CLA:HHC  | 22:C:1030:CLA:HBB1 | 1.33                     | 1.10              |
| 22:a:6006:CLA:H172 | 25:d:6050:BCR:C28  | 1.80                     | 1.10              |
| 26:a:6063:LHG:H291 | 22:c:6032:CLA:H72  | 1.30                     | 1.10              |
| 22:b:6022:CLA:C14  | 22:b:6022:CLA:C9   | 2.30                     | 1.10              |
| 22:c:6025:CLA:H12  | 22:c:6025:CLA:HBB  | 1.22                     | 1.10              |
| 25:k:6052:BCR:C38  | 25:k:6052:BCR:C37  | 2.30                     | 1.10              |
| 2:B:174:LEU:HD22   | 2:B:312:TYR:OH     | 1.48                     | 1.09              |
| 2:b:5005:TRP:HA    | 2:b:5008:VAL:CG1   | 1.82                     | 1.09              |
| 22:b:6021:CLA:C1A  | 22:b:6021:CLA:CED  | 2.30                     | 1.09              |
| 22:c:6025:CLA:C4   | 22:c:6025:CLA:C2B  | 2.30                     | 1.09              |
| 22:d:6005:CLA:H122 | 22:d:6005:CLA:H91  | 1.10                     | 1.09              |
| 25:d:6050:BCR:H23C | 25:d:6050:BCR:H383 | 1.11                     | 1.09              |
| 22:b:6009:CLA:HBD  | 22:b:6010:CLA:HBB1 | 1.11                     | 1.09              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6022:CLA:C9   | 22:b:6022:CLA:H142 | 1.82                     | 1.09              |
| 25:b:6047:BCR:HC8  | 25:b:6047:BCR:C33  | 1.83                     | 1.09              |
| 22:c:6030:CLA:HHD  | 22:c:6030:CLA:CBC  | 1.82                     | 1.09              |
| 22:c:6030:CLA:HHC  | 22:c:6030:CLA:HBB1 | 1.33                     | 1.09              |
| 25:h:6049:BCR:H392 | 25:h:6049:BCR:C23  | 1.76                     | 1.09              |
| 22:C:1035:CLA:HHC  | 22:C:1035:CLA:HBB1 | 1.30                     | 1.09              |
| 25:C:1052:BCR:C38  | 25:C:1052:BCR:C37  | 2.30                     | 1.09              |
| 1:a:5205:VAL:HA    | 1:a:5279:ARG:NH1   | 1.66                     | 1.09              |
| 22:a:6006:CLA:HBC3 | 22:a:6006:CLA:HHD  | 1.24                     | 1.09              |
| 23:a:6038:PHO:H202 | 22:d:6005:CLA:HMB1 | 1.33                     | 1.09              |
| 22:b:6015:CLA:H41  | 22:b:6015:CLA:C7   | 1.76                     | 1.09              |
| 23:d:6039:PHO:HBA2 | 23:d:6039:PHO:HMA2 | 1.11                     | 1.09              |
| 22:k:6034:CLA:HBC3 | 22:k:6034:CLA:HHD  | 1.31                     | 1.09              |
| 22:B:1022:CLA:C14  | 22:B:1022:CLA:C6   | 2.31                     | 1.09              |
| 3:C:49:LEU:CD2     | 3:C:52:ALA:H       | 1.66                     | 1.09              |
| 3:C:171:GLY:HA2    | 3:C:174:LEU:HB2    | 1.35                     | 1.09              |
| 22:D:1008:CLA:C14  | 22:D:1008:CLA:C19  | 2.30                     | 1.09              |
| 22:D:1008:CLA:HHC  | 22:D:1008:CLA:HBB1 | 1.29                     | 1.09              |
| 22:a:6006:CLA:H172 | 25:d:6050:BCR:C27  | 1.83                     | 1.09              |
| 22:b:6011:CLA:CED  | 22:b:6012:CLA:CED  | 2.24                     | 1.09              |
| 22:c:6025:CLA:H122 | 25:c:6054:BCR:H351 | 1.12                     | 1.09              |
| 22:c:6033:CLA:H143 | 22:c:6033:CLA:H171 | 1.10                     | 1.09              |
| 22:B:1009:CLA:CGD  | 22:B:1009:CLA:CBA  | 2.30                     | 1.09              |
| 22:B:1009:CLA:C14  | 22:B:1009:CLA:C8   | 2.30                     | 1.09              |
| 22:B:1014:CLA:C4   | 22:B:1014:CLA:H72  | 1.82                     | 1.09              |
| 22:B:1016:CLA:H2   | 22:H:1017:CLA:C9   | 1.81                     | 1.09              |
| 22:B:1018:CLA:HBB1 | 22:B:1018:CLA:HHC  | 1.31                     | 1.09              |
| 22:C:1025:CLA:H122 | 25:C:1054:BCR:H351 | 1.12                     | 1.09              |
| 22:C:1037:CLA:HHC  | 22:C:1037:CLA:HBB1 | 1.31                     | 1.09              |
| 25:C:1052:BCR:C26  | 25:C:1052:BCR:C37  | 2.30                     | 1.09              |
| 4:D:201:VAL:HG23   | 22:D:1004:CLA:HMB2 | 1.27                     | 1.09              |
| 23:D:1039:PHO:HBA2 | 23:D:1039:PHO:HMA2 | 1.11                     | 1.09              |
| 25:D:1050:BCR:H372 | 28:D:1059:MGE:H3A1 | 1.16                     | 1.09              |
| 11:L:26:VAL:HG21   | 28:L:1061:MGE:H232 | 1.35                     | 1.09              |
| 1:a:5205:VAL:HB    | 1:a:5279:ARG:HH12  | 0.98                     | 1.09              |
| 22:a:6003:CLA:H142 | 23:a:6038:PHO:H8   | 1.17                     | 1.09              |
| 2:B:5:TRP:HA       | 2:B:8:VAL:CG1      | 1.82                     | 1.08              |
| 3:C:263:ALA:HB3    | 3:C:264:PHE:CE2    | 1.89                     | 1.08              |
| 22:C:1025:CLA:C4   | 22:C:1025:CLA:C2B  | 2.30                     | 1.08              |
| 22:C:1030:CLA:HHD  | 22:C:1030:CLA:CBC  | 1.82                     | 1.08              |
| 25:T:6046:BCR:HC8  | 25:T:6046:BCR:H331 | 1.09                     | 1.08              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:a:6006:CLA:H172 | 25:d:6050:BCR:H282 | 1.29                     | 1.08              |
| 22:b:6009:CLA:C14  | 22:b:6009:CLA:C8   | 2.30                     | 1.08              |
| 22:b:6021:CLA:H102 | 22:b:6021:CLA:C14  | 1.83                     | 1.08              |
| 22:c:6025:CLA:H151 | 22:c:6031:CLA:C9   | 1.80                     | 1.08              |
| 22:C:1027:CLA:H171 | 22:C:1027:CLA:H122 | 1.10                     | 1.08              |
| 29:C:1057:DGD:HB81 | 28:D:1059:MGE:H8B2 | 1.32                     | 1.08              |
| 22:K:1034:CLA:HHD  | 22:K:1034:CLA:HBC3 | 1.31                     | 1.08              |
| 26:a:6063:LHG:H291 | 22:c:6032:CLA:C7   | 1.82                     | 1.08              |
| 2:b:5005:TRP:HA    | 2:b:5008:VAL:HG13  | 1.33                     | 1.08              |
| 22:b:6009:CLA:CGD  | 22:b:6009:CLA:CBA  | 2.30                     | 1.08              |
| 22:d:6008:CLA:HBB1 | 22:d:6008:CLA:HHC  | 1.29                     | 1.08              |
| 22:B:1020:CLA:HED1 | 22:B:1021:CLA:HMB2 | 1.32                     | 1.08              |
| 22:B:1021:CLA:C2A  | 22:B:1021:CLA:CED  | 2.30                     | 1.08              |
| 29:c:6057:DGD:HB81 | 28:d:6059:MGE:H8B2 | 1.33                     | 1.08              |
| 22:d:6004:CLA:HHC  | 22:d:6004:CLA:HBB1 | 1.31                     | 1.08              |
| 11:l:5026:VAL:HG21 | 28:l:6061:MGE:H232 | 1.35                     | 1.08              |
| 29:C:1056:DGD:HE5  | 29:C:1056:DGD:C6D  | 1.83                     | 1.08              |
| 29:C:1056:DGD:HD62 | 29:C:1056:DGD:C5E  | 1.84                     | 1.08              |
| 4:D:160:TYR:CZ     | 27:D:1068:IOD:I    | 2.77                     | 1.08              |
| 22:D:1004:CLA:HBB1 | 22:D:1004:CLA:HHC  | 1.31                     | 1.08              |
| 28:D:1059:MGE:H251 | 28:D:1059:MGE:H211 | 1.15                     | 1.08              |
| 29:c:6056:DGD:HE5  | 29:c:6056:DGD:C6D  | 1.83                     | 1.08              |
| 25:k:6052:BCR:C26  | 25:k:6052:BCR:C37  | 2.30                     | 1.08              |
| 22:A:1006:CLA:H172 | 25:D:1050:BCR:C27  | 1.83                     | 1.08              |
| 22:B:1021:CLA:C1A  | 22:B:1021:CLA:CED  | 2.30                     | 1.08              |
| 22:B:1022:CLA:C14  | 22:B:1022:CLA:C9   | 2.30                     | 1.08              |
| 22:C:1025:CLA:H122 | 25:C:1054:BCR:C35  | 1.84                     | 1.08              |
| 22:c:6030:CLA:H172 | 22:c:6030:CLA:H121 | 1.10                     | 1.08              |
| 22:B:1018:CLA:H101 | 22:B:1023:CLA:HAA1 | 1.36                     | 1.07              |
| 22:B:1021:CLA:C14  | 22:B:1021:CLA:H102 | 1.83                     | 1.07              |
| 22:C:1030:CLA:HHD  | 22:C:1030:CLA:HBC2 | 1.32                     | 1.07              |
| 25:C:1054:BCR:H403 | 25:C:1054:BCR:C23  | 1.74                     | 1.07              |
| 29:C:1057:DGD:HAF2 | 28:D:1059:MGE:H222 | 1.08                     | 1.07              |
| 13:O:179:THR:HG22  | 13:O:180:ALA:H     | 1.11                     | 1.07              |
| 22:b:6022:CLA:H122 | 22:b:6022:CLA:H91  | 1.11                     | 1.07              |
| 3:c:5263:ALA:HB3   | 3:c:5264:PHE:CE2   | 1.89                     | 1.07              |
| 22:c:6026:CLA:H122 | 22:c:6026:CLA:H71  | 1.33                     | 1.07              |
| 29:c:6056:DGD:HD62 | 29:c:6056:DGD:C5E  | 1.84                     | 1.07              |
| 24:A:1043:PQ9:H451 | 28:D:1059:MGE:H101 | 1.08                     | 1.07              |
| 26:A:1063:LHG:H291 | 22:C:1032:CLA:H72  | 1.33                     | 1.07              |
| 22:B:1009:CLA:HHC  | 22:B:1009:CLA:HBB1 | 1.35                     | 1.07              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:Z:1053:BCR:H23C | 25:Z:1053:BCR:H383 | 1.11                     | 1.07              |
| 22:b:6014:CLA:C4   | 22:b:6014:CLA:H72  | 1.82                     | 1.07              |
| 22:B:1012:CLA:C2D  | 22:B:1020:CLA:H201 | 1.84                     | 1.07              |
| 22:B:1022:CLA:HBC3 | 22:B:1022:CLA:H92  | 1.07                     | 1.07              |
| 22:B:1023:CLA:H13  | 22:B:1024:CLA:HMA3 | 1.18                     | 1.07              |
| 22:C:1026:CLA:CBA  | 22:C:1027:CLA:HAC1 | 1.85                     | 1.07              |
| 22:b:6012:CLA:C2D  | 22:b:6020:CLA:H201 | 1.84                     | 1.07              |
| 3:c:5049:LEU:CD2   | 3:c:5052:ALA:H     | 1.66                     | 1.07              |
| 25:z:6053:BCR:H23C | 25:z:6053:BCR:H383 | 1.11                     | 1.07              |
| 3:C:417:VAL:HG12   | 16:V:68:VAL:HB     | 1.35                     | 1.07              |
| 3:C:417:VAL:HG11   | 16:V:68:VAL:CG1    | 1.84                     | 1.07              |
| 22:C:1026:CLA:HBA1 | 22:C:1027:CLA:CAC  | 1.85                     | 1.07              |
| 23:D:1039:PHO:CMA  | 23:D:1039:PHO:CBA  | 2.30                     | 1.07              |
| 1:a:5337:HIS:O     | 4:d:5351:ALA:HB2   | 1.54                     | 1.07              |
| 22:b:6009:CLA:C8   | 22:b:6009:CLA:H143 | 1.84                     | 1.07              |
| 22:b:6010:CLA:H112 | 22:b:6010:CLA:C16  | 1.71                     | 1.07              |
| 22:b:6022:CLA:C14  | 22:b:6022:CLA:C6   | 2.31                     | 1.07              |
| 13:o:5179:THR:HG22 | 13:o:5180:ALA:H    | 1.12                     | 1.07              |
| 2:B:362:PHE:CE1    | 27:D:1068:IOD:I    | 2.78                     | 1.07              |
| 22:B:1009:CLA:HAA1 | 22:B:1009:CLA:O2D  | 1.55                     | 1.07              |
| 22:B:1009:CLA:HBD  | 22:B:1010:CLA:HBB1 | 1.11                     | 1.07              |
| 22:B:1010:CLA:HBD  | 22:B:1010:CLA:H12  | 1.35                     | 1.07              |
| 22:B:1011:CLA:CGA  | 22:B:1011:CLA:C3A  | 2.33                     | 1.07              |
| 22:C:1027:CLA:C12  | 22:C:1027:CLA:C17  | 2.31                     | 1.07              |
| 22:b:6011:CLA:CMD  | 22:b:6013:CLA:H42  | 1.82                     | 1.07              |
| 3:c:5417:VAL:HG11  | 16:v:5068:VAL:CG1  | 1.84                     | 1.07              |
| 22:B:1012:CLA:C2D  | 22:B:1020:CLA:C20  | 2.33                     | 1.06              |
| 22:B:1012:CLA:HBB1 | 22:B:1015:CLA:CBB  | 1.85                     | 1.06              |
| 22:B:1022:CLA:H122 | 22:B:1022:CLA:H91  | 1.11                     | 1.06              |
| 5:E:8:ARG:HE       | 6:F:13:TYR:HB2     | 1.18                     | 1.06              |
| 22:K:1034:CLA:C4   | 22:K:1034:CLA:CGA  | 2.33                     | 1.06              |
| 25:T:6048:BCR:C40  | 25:T:6048:BCR:C37  | 2.30                     | 1.06              |
| 22:b:6009:CLA:HED3 | 22:b:6009:CLA:H2A  | 1.09                     | 1.06              |
| 22:c:6025:CLA:H42  | 22:c:6025:CLA:HMB1 | 1.09                     | 1.06              |
| 22:c:6026:CLA:CBA  | 22:c:6027:CLA:HAC1 | 1.85                     | 1.06              |
| 29:c:6056:DGD:C6D  | 29:c:6056:DGD:HE3  | 1.84                     | 1.06              |
| 10:k:5032:PHE:HE1  | 25:k:6052:BCR:C21  | 1.67                     | 1.06              |
| 22:A:1003:CLA:H42  | 23:A:1038:PHO:C4B  | 1.85                     | 1.06              |
| 22:B:1009:CLA:CED  | 22:B:1009:CLA:CAA  | 2.30                     | 1.06              |
| 3:c:5049:LEU:HD21  | 3:c:5052:ALA:HB2   | 1.37                     | 1.06              |
| 22:c:6025:CLA:H122 | 25:c:6054:BCR:C35  | 1.84                     | 1.06              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1011:CLA:CED  | 22:B:1012:CLA:CED  | 2.25                     | 1.06              |
| 29:B:1058:DGD:HBT1 | 29:B:1058:DGD:C6B  | 1.84                     | 1.06              |
| 28:D:1062:MGE:O1B  | 28:D:1062:MGE:H3G2 | 1.55                     | 1.06              |
| 22:a:6003:CLA:H42  | 23:a:6038:PHO:C4B  | 1.85                     | 1.06              |
| 22:b:6009:CLA:CED  | 22:b:6009:CLA:CAA  | 2.30                     | 1.06              |
| 24:A:1043:PQ9:H451 | 28:D:1059:MGE:CAA  | 1.86                     | 1.06              |
| 22:B:1009:CLA:C8   | 22:B:1009:CLA:H143 | 1.84                     | 1.06              |
| 22:C:1025:CLA:H42  | 22:C:1025:CLA:HMB1 | 1.09                     | 1.06              |
| 25:K:1051:BCR:H353 | 18:Y:32:GLY:HA3    | 1.32                     | 1.06              |
| 22:b:6010:CLA:H162 | 22:b:6010:CLA:H111 | 1.34                     | 1.06              |
| 22:b:6022:CLA:HBC3 | 22:b:6022:CLA:H92  | 1.07                     | 1.06              |
| 29:b:6058:DGD:HBT1 | 29:b:6058:DGD:C6B  | 1.84                     | 1.06              |
| 3:c:5049:LEU:CD2   | 3:c:5052:ALA:HB2   | 1.86                     | 1.06              |
| 22:c:6026:CLA:HBA1 | 22:c:6027:CLA:CAC  | 1.85                     | 1.06              |
| 22:B:1009:CLA:HED3 | 22:B:1009:CLA:H2A  | 1.08                     | 1.06              |
| 22:B:1022:CLA:H62  | 22:B:1022:CLA:H142 | 1.06                     | 1.06              |
| 3:C:32:GLY:HA3     | 3:C:41:ARG:HD3     | 1.37                     | 1.06              |
| 22:C:1033:CLA:H143 | 22:C:1033:CLA:H171 | 1.10                     | 1.06              |
| 22:D:1008:CLA:H143 | 22:D:1008:CLA:C18  | 1.86                     | 1.06              |
| 28:D:1062:MGE:H1G1 | 11:L:19:LEU:HD21   | 1.37                     | 1.06              |
| 1:a:5258:LEU:HD12  | 4:d:5128:ARG:HH21  | 1.14                     | 1.06              |
| 2:b:5005:TRP:CZ2   | 28:l:6061:MGE:H2A2 | 1.90                     | 1.06              |
| 22:b:6012:CLA:HBB1 | 22:b:6015:CLA:CBB  | 1.85                     | 1.06              |
| 25:b:6047:BCR:C40  | 25:b:6047:BCR:C37  | 2.30                     | 1.06              |
| 22:k:6034:CLA:C4   | 22:k:6034:CLA:CGA  | 2.33                     | 1.06              |
| 3:C:49:LEU:HD22    | 3:C:52:ALA:N       | 1.71                     | 1.05              |
| 25:a:6044:BCR:C40  | 25:a:6044:BCR:C37  | 2.30                     | 1.05              |
| 22:b:6009:CLA:HAA1 | 22:b:6009:CLA:O2D  | 1.55                     | 1.05              |
| 22:d:6008:CLA:C14  | 22:d:6008:CLA:C19  | 2.30                     | 1.05              |
| 2:B:362:PHE:HE1    | 27:D:1068:IOD:I    | 2.09                     | 1.05              |
| 3:C:49:LEU:CD2     | 3:C:52:ALA:HB2     | 1.86                     | 1.05              |
| 3:C:50:LEU:HD21    | 3:C:54:VAL:CG2     | 1.86                     | 1.05              |
| 22:D:1008:CLA:CMA  | 22:D:1008:CLA:CBA  | 2.30                     | 1.05              |
| 22:b:6010:CLA:H12  | 22:b:6010:CLA:HBD  | 1.35                     | 1.05              |
| 3:c:5050:LEU:HD21  | 3:c:5054:VAL:CG2   | 1.86                     | 1.05              |
| 3:c:5275:SER:HB3   | 22:c:6033:CLA:HED1 | 1.34                     | 1.05              |
| 22:d:6005:CLA:H91  | 22:d:6005:CLA:C12  | 1.83                     | 1.05              |
| 2:B:5:TRP:CZ2      | 28:L:1061:MGE:H2A2 | 1.90                     | 1.05              |
| 25:B:1047:BCR:C39  | 25:B:1047:BCR:C37  | 2.30                     | 1.05              |
| 29:C:1056:DGD:C6D  | 29:C:1056:DGD:HE3  | 1.84                     | 1.05              |
| 22:c:6025:CLA:CMB  | 22:c:6025:CLA:C4   | 2.34                     | 1.05              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B:1048:BCR:C39  | 25:B:1048:BCR:C37  | 2.30                     | 1.05              |
| 3:C:42:LEU:HD11    | 3:C:49:LEU:CD1     | 1.86                     | 1.05              |
| 3:C:343:ARG:HH12   | 3:C:348:GLU:CG     | 1.68                     | 1.05              |
| 22:C:1025:CLA:CMB  | 22:C:1025:CLA:C4   | 2.34                     | 1.05              |
| 4:D:246:MET:HE3    | 4:D:264:LYS:HG2    | 1.39                     | 1.05              |
| 22:D:1005:CLA:H122 | 22:D:1005:CLA:H91  | 1.10                     | 1.05              |
| 16:V:103:LYS:HD2   | 16:V:121:LEU:HD12  | 1.37                     | 1.05              |
| 3:c:5343:ARG:HH12  | 3:c:5348:GLU:CG    | 1.68                     | 1.05              |
| 25:B:1047:BCR:H331 | 25:B:1047:BCR:HC8  | 1.37                     | 1.05              |
| 22:D:1005:CLA:H91  | 22:D:1005:CLA:C12  | 1.83                     | 1.05              |
| 16:V:103:LYS:HD2   | 16:V:121:LEU:CD1   | 1.87                     | 1.05              |
| 25:t:1046:BCR:HC8  | 25:t:1046:BCR:H331 | 1.09                     | 1.05              |
| 22:b:6011:CLA:CGA  | 22:b:6011:CLA:C3A  | 2.32                     | 1.04              |
| 22:b:6012:CLA:C2D  | 22:b:6020:CLA:C20  | 2.33                     | 1.04              |
| 3:c:5049:LEU:HD22  | 3:c:5052:ALA:N     | 1.71                     | 1.04              |
| 29:c:6057:DGD:HAF2 | 28:d:6059:MGE:H222 | 1.08                     | 1.04              |
| 23:A:1038:PHO:H202 | 22:D:1005:CLA:HMB1 | 1.33                     | 1.04              |
| 25:B:1047:BCR:H24C | 25:t:1046:BCR:H353 | 1.37                     | 1.04              |
| 25:H:1049:BCR:H392 | 25:H:1049:BCR:C23  | 1.76                     | 1.04              |
| 10:K:39:VAL:CG2    | 18:Y:36:ILE:HD11   | 1.86                     | 1.04              |
| 3:c:5417:VAL:HG12  | 16:v:5068:VAL:HB   | 1.35                     | 1.04              |
| 22:d:6008:CLA:C14  | 22:d:6008:CLA:C18  | 2.36                     | 1.04              |
| 5:e:5008:ARG:HE    | 6:f:5013:TYR:HB2   | 1.18                     | 1.04              |
| 2:B:4:PRO:HG2      | 2:B:7:ARG:HG3      | 1.38                     | 1.04              |
| 22:B:1009:CLA:H102 | 22:B:1009:CLA:H142 | 1.39                     | 1.04              |
| 25:B:1047:BCR:HC8  | 25:B:1047:BCR:C33  | 1.82                     | 1.04              |
| 22:D:1008:CLA:C14  | 22:D:1008:CLA:C18  | 2.36                     | 1.04              |
| 4:d:5057:SER:HB2   | 4:d:5079:SER:HB3   | 1.37                     | 1.04              |
| 23:D:1039:PHO:CMA  | 22:D:1004:CLA:H143 | 1.87                     | 1.04              |
| 14:T:18:PHE:HA     | 25:T:6046:BCR:H332 | 1.36                     | 1.04              |
| 28:d:6062:MGE:O1B  | 28:d:6062:MGE:H3G2 | 1.55                     | 1.04              |
| 22:B:1010:CLA:H162 | 22:B:1010:CLA:H111 | 1.34                     | 1.04              |
| 24:a:6043:PQ9:H451 | 28:d:6059:MGE:H101 | 1.08                     | 1.04              |
| 22:b:6022:CLA:C9   | 22:b:6022:CLA:C12  | 2.32                     | 1.04              |
| 23:d:6039:PHO:CMA  | 22:d:6004:CLA:H143 | 1.87                     | 1.04              |
| 3:C:49:LEU:HD21    | 3:C:52:ALA:HB2     | 1.37                     | 1.03              |
| 3:C:275:SER:HB3    | 22:C:1033:CLA:HED1 | 1.34                     | 1.03              |
| 22:C:1030:CLA:H172 | 22:C:1030:CLA:H121 | 1.10                     | 1.03              |
| 4:D:57:SER:HB2     | 4:D:79:SER:HB3     | 1.37                     | 1.03              |
| 24:a:6043:PQ9:H451 | 28:d:6059:MGE:CAA  | 1.86                     | 1.03              |
| 22:d:6008:CLA:H143 | 22:d:6008:CLA:C18  | 1.86                     | 1.03              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:v:5098:LEU:HD22 | 16:v:5098:LEU:H    | 1.20                     | 1.03              |
| 22:A:1006:CLA:HHC  | 22:A:1006:CLA:HBB1 | 1.38                     | 1.03              |
| 22:B:1015:CLA:CBC  | 25:B:1045:BCR:H342 | 1.88                     | 1.03              |
| 29:C:1057:DGD:HB2  | 29:C:1057:DGD:HBG2 | 1.35                     | 1.03              |
| 22:K:1034:CLA:H102 | 22:K:1034:CLA:H143 | 1.40                     | 1.03              |
| 25:T:6048:BCR:C39  | 25:T:6048:BCR:C37  | 2.30                     | 1.03              |
| 2:b:5004:PRO:HG2   | 2:b:5007:ARG:HG3   | 1.38                     | 1.03              |
| 22:k:6034:CLA:H102 | 22:k:6034:CLA:H143 | 1.40                     | 1.03              |
| 22:A:1003:CLA:H42  | 23:A:1038:PHO:C1B  | 1.88                     | 1.03              |
| 22:B:1021:CLA:C10  | 22:B:1021:CLA:C14  | 2.34                     | 1.03              |
| 3:C:49:LEU:HD12    | 3:C:49:LEU:H       | 1.23                     | 1.03              |
| 22:b:6021:CLA:C2A  | 22:b:6021:CLA:CED  | 2.30                     | 1.03              |
| 22:d:6008:CLA:HBA1 | 22:d:6008:CLA:HMA2 | 1.06                     | 1.03              |
| 7:h:5013:PRO:HG2   | 7:h:5014:LEU:HD12  | 1.39                     | 1.03              |
| 22:B:1015:CLA:HAC2 | 25:t:1046:BCR:C28  | 1.89                     | 1.03              |
| 31:F:1040:HEM:HBA2 | 31:F:1040:HEM:HMA1 | 1.05                     | 1.03              |
| 2:b:5174:LEU:H     | 2:b:5174:LEU:HD13  | 1.21                     | 1.03              |
| 22:b:6009:CLA:H142 | 22:b:6009:CLA:C10  | 1.89                     | 1.03              |
| 22:c:6027:CLA:H171 | 22:c:6027:CLA:H122 | 1.10                     | 1.03              |
| 2:B:174:LEU:HD13   | 2:B:174:LEU:H      | 1.21                     | 1.03              |
| 3:c:5049:LEU:HB3   | 3:c:5133:ALA:HA    | 1.40                     | 1.03              |
| 3:c:5050:LEU:C     | 3:c:5050:LEU:CD2   | 2.30                     | 1.03              |
| 25:c:6054:BCR:H403 | 25:c:6054:BCR:C23  | 1.75                     | 1.03              |
| 2:B:105:GLY:CA     | 25:B:1047:BCR:H401 | 1.88                     | 1.02              |
| 22:B:1013:CLA:H122 | 22:B:1018:CLA:H42  | 1.38                     | 1.02              |
| 22:B:1021:CLA:OBD  | 22:B:1022:CLA:HHC  | 1.59                     | 1.02              |
| 22:D:1005:CLA:C12  | 22:D:1005:CLA:C9   | 2.36                     | 1.02              |
| 22:D:1008:CLA:HBA1 | 22:D:1008:CLA:HMA2 | 1.06                     | 1.02              |
| 22:b:6011:CLA:O1D  | 22:b:6013:CLA:H11  | 1.58                     | 1.02              |
| 22:b:6022:CLA:H62  | 22:b:6022:CLA:H142 | 1.06                     | 1.02              |
| 4:d:5091:LEU:HA    | 22:d:6008:CLA:HED1 | 1.41                     | 1.02              |
| 22:d:6005:CLA:C12  | 22:d:6005:CLA:C9   | 2.36                     | 1.02              |
| 22:B:1019:CLA:H93  | 28:L:1061:MGE:H9A2 | 1.41                     | 1.02              |
| 25:T:6046:BCR:C28  | 22:b:6015:CLA:HAC2 | 1.89                     | 1.02              |
| 22:a:6007:CLA:C4   | 22:c:6029:CLA:H191 | 1.89                     | 1.02              |
| 2:b:5105:GLY:CA    | 25:b:6047:BCR:H401 | 1.88                     | 1.02              |
| 2:b:5456:ALA:HB1   | 29:b:6058:DGD:HBV1 | 1.41                     | 1.02              |
| 22:b:6009:CLA:HHC  | 22:b:6009:CLA:HBB1 | 1.35                     | 1.02              |
| 22:b:6015:CLA:CBC  | 25:b:6045:BCR:H342 | 1.88                     | 1.02              |
| 22:b:6023:CLA:HED2 | 22:b:6024:CLA:HBB1 | 1.03                     | 1.02              |
| 22:c:6030:CLA:C12  | 22:c:6030:CLA:C17  | 2.30                     | 1.02              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:d:6005:CLA:H122 | 22:d:6005:CLA:C9   | 1.90                     | 1.02              |
| 28:d:6062:MGE:H1G1 | 11:l:5019:LEU:HD21 | 1.37                     | 1.02              |
| 10:k:5024:VAL:HG21 | 18:y:5025:ILE:HG22 | 1.41                     | 1.02              |
| 20:z:5055:GLY:HA2  | 25:z:6053:BCR:C31  | 1.88                     | 1.02              |
| 22:A:1007:CLA:C4   | 22:C:1029:CLA:H191 | 1.89                     | 1.02              |
| 22:B:1014:CLA:H41  | 22:B:1014:CLA:H72  | 1.03                     | 1.02              |
| 3:C:343:ARG:NH1    | 3:C:348:GLU:CG     | 2.21                     | 1.02              |
| 20:Z:55:GLY:HA2    | 25:Z:1053:BCR:C31  | 1.88                     | 1.02              |
| 22:c:6029:CLA:H42  | 22:c:6029:CLA:NC   | 1.74                     | 1.02              |
| 29:c:6057:DGD:HB2  | 29:c:6057:DGD:HBG2 | 1.35                     | 1.02              |
| 26:A:1063:LHG:H161 | 26:A:1063:LHG:H122 | 1.42                     | 1.02              |
| 2:B:7:ARG:HG2      | 2:B:7:ARG:HH11     | 1.20                     | 1.02              |
| 3:C:265:ILE:HD11   | 3:C:452:ALA:HB2    | 1.05                     | 1.02              |
| 22:C:1033:CLA:HMA2 | 22:K:1034:CLA:HAC1 | 1.42                     | 1.02              |
| 25:T:6046:BCR:H353 | 25:b:6047:BCR:H24C | 1.37                     | 1.02              |
| 22:a:6003:CLA:H42  | 23:a:6038:PHO:C1B  | 1.88                     | 1.02              |
| 25:b:6047:BCR:HC8  | 25:b:6047:BCR:H331 | 1.37                     | 1.02              |
| 3:c:5264:PHE:N     | 3:c:5264:PHE:HD2   | 1.57                     | 1.02              |
| 22:B:1011:CLA:O1D  | 22:B:1013:CLA:H11  | 1.58                     | 1.02              |
| 25:B:1047:BCR:C40  | 25:B:1047:BCR:C37  | 2.30                     | 1.02              |
| 4:D:37:LEU:HD22    | 4:D:128:ARG:HD3    | 1.41                     | 1.02              |
| 16:V:98:LEU:HD22   | 16:V:98:LEU:H      | 1.20                     | 1.02              |
| 1:a:5279:ARG:HH21  | 23:a:6038:PHO:HMC2 | 1.19                     | 1.02              |
| 2:b:5326:ARG:HH11  | 4:d:5297:ASP:HA    | 1.24                     | 1.02              |
| 4:d:5246:MET:HE3   | 4:d:5264:LYS:HG2   | 1.39                     | 1.02              |
| 22:d:6008:CLA:H193 | 22:d:6008:CLA:H143 | 1.33                     | 1.02              |
| 25:k:6052:BCR:C37  | 25:k:6052:BCR:H383 | 1.90                     | 1.02              |
| 25:A:1044:BCR:C39  | 25:A:1044:BCR:C37  | 2.30                     | 1.01              |
| 25:A:1044:BCR:C40  | 25:A:1044:BCR:C37  | 2.30                     | 1.01              |
| 2:B:105:GLY:HA3    | 25:B:1047:BCR:H401 | 1.39                     | 1.01              |
| 3:C:46:SER:HB2     | 3:C:141:GLU:CB     | 1.90                     | 1.01              |
| 3:c:5032:GLY:HA3   | 3:c:5041:ARG:HD3   | 1.37                     | 1.01              |
| 3:c:5046:SER:HB2   | 3:c:5141:GLU:CB    | 1.90                     | 1.01              |
| 4:d:5250:ASN:HB2   | 4:d:5260:ALA:HB1   | 1.40                     | 1.01              |
| 22:B:1023:CLA:HED2 | 22:B:1024:CLA:HBB1 | 1.03                     | 1.01              |
| 4:D:250:ASN:HB2    | 4:D:260:ALA:HB1    | 1.40                     | 1.01              |
| 22:a:6006:CLA:HBB1 | 22:a:6006:CLA:HHC  | 1.38                     | 1.01              |
| 2:b:5105:GLY:HA3   | 25:b:6047:BCR:H401 | 1.39                     | 1.01              |
| 22:b:6016:CLA:C5   | 22:h:6017:CLA:H112 | 1.91                     | 1.01              |
| 22:b:6018:CLA:H101 | 22:b:6023:CLA:HAA1 | 1.36                     | 1.01              |
| 22:B:1019:CLA:H93  | 28:L:1061:MGE:C9A  | 1.90                     | 1.01              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:264:PHE:N      | 3:C:264:PHE:HD2    | 1.57                     | 1.01              |
| 22:C:1029:CLA:H42  | 22:C:1029:CLA:NC   | 1.74                     | 1.01              |
| 4:D:267:LEU:HD22   | 4:D:268:HIS:ND1    | 1.74                     | 1.01              |
| 26:a:6063:LHG:H292 | 22:c:6032:CLA:H52  | 1.40                     | 1.01              |
| 2:b:5007:ARG:HG2   | 2:b:5007:ARG:HH11  | 1.20                     | 1.01              |
| 22:b:6009:CLA:H142 | 22:b:6009:CLA:H102 | 1.39                     | 1.01              |
| 22:b:6013:CLA:H122 | 22:b:6018:CLA:H42  | 1.38                     | 1.01              |
| 22:b:6014:CLA:H41  | 22:b:6014:CLA:H72  | 1.03                     | 1.01              |
| 22:c:6027:CLA:C12  | 22:c:6027:CLA:C17  | 2.31                     | 1.01              |
| 22:c:6033:CLA:HMA2 | 22:k:6034:CLA:HAC1 | 1.42                     | 1.01              |
| 2:B:326:ARG:HH11   | 4:D:297:ASP:HA     | 1.24                     | 1.01              |
| 3:C:229:ASN:HD22   | 3:C:229:ASN:H      | 1.03                     | 1.01              |
| 10:K:24:VAL:HG21   | 18:Y:25:ILE:HG22   | 1.41                     | 1.01              |
| 22:b:6019:CLA:H93  | 28:l:6061:MGE:C9A  | 1.90                     | 1.01              |
| 3:c:5171:GLY:HA2   | 3:c:5174:LEU:HB2   | 1.35                     | 1.01              |
| 4:d:5261:PHE:CZ    | 4:d:5267:LEU:HA    | 1.96                     | 1.01              |
| 31:f:6040:HEM:HBA2 | 31:f:6040:HEM:HMA1 | 1.05                     | 1.01              |
| 4:D:261:PHE:CZ     | 4:D:267:LEU:HA     | 1.96                     | 1.01              |
| 22:D:1005:CLA:H122 | 22:D:1005:CLA:C9   | 1.90                     | 1.01              |
| 25:a:6044:BCR:C39  | 25:a:6044:BCR:C37  | 2.30                     | 1.01              |
| 2:b:5075:TRP:NE1   | 2:b:5094:GLU:HB2   | 1.76                     | 1.01              |
| 3:c:5265:ILE:HD11  | 3:c:5452:ALA:HB2   | 1.05                     | 1.01              |
| 22:c:6027:CLA:H152 | 25:z:6053:BCR:H332 | 1.42                     | 1.01              |
| 22:B:1021:CLA:HED2 | 22:B:1021:CLA:CHA  | 1.91                     | 1.00              |
| 1:a:5212:CYS:HB2   | 4:d:5211:CYS:HB2   | 1.43                     | 1.00              |
| 22:d:6008:CLA:CMA  | 22:d:6008:CLA:CBA  | 2.30                     | 1.00              |
| 1:A:60:ILE:HD11    | 1:A:83:VAL:HB      | 1.41                     | 1.00              |
| 26:A:1063:LHG:H292 | 22:C:1032:CLA:H52  | 1.41                     | 1.00              |
| 22:B:1009:CLA:HMB3 | 25:H:1049:BCR:H271 | 1.01                     | 1.00              |
| 7:H:13:PRO:HG2     | 7:H:14:LEU:HD12    | 1.39                     | 1.00              |
| 3:c:5049:LEU:H     | 3:c:5049:LEU:HD12  | 1.22                     | 1.00              |
| 3:c:5265:ILE:HD11  | 3:c:5452:ALA:CB    | 1.91                     | 1.00              |
| 2:B:456:ALA:HB1    | 29:B:1058:DGD:HBV1 | 1.41                     | 1.00              |
| 22:B:1022:CLA:C9   | 22:B:1022:CLA:C12  | 2.32                     | 1.00              |
| 3:C:167:VAL:HG12   | 3:C:168:LEU:HD12   | 1.44                     | 1.00              |
| 4:D:265:ARG:HH11   | 4:D:265:ARG:HG3    | 1.23                     | 1.00              |
| 2:b:5149:LEU:CG    | 22:b:6011:CLA:HBC1 | 1.91                     | 1.00              |
| 2:b:5324:LEU:HA    | 4:d:5293:LEU:HD22  | 1.43                     | 1.00              |
| 22:C:1027:CLA:C17  | 22:C:1027:CLA:H121 | 1.91                     | 1.00              |
| 22:b:6021:CLA:HED2 | 22:b:6021:CLA:CHA  | 1.91                     | 1.00              |
| 12:m:5029:THR:O    | 12:m:5032:GLN:HG2  | 1.61                     | 1.00              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:54:ALA:HB2     | 1:A:72:LEU:HD12    | 1.42                     | 1.00              |
| 22:B:1016:CLA:C5   | 22:H:1017:CLA:H112 | 1.91                     | 1.00              |
| 10:K:39:VAL:HG23   | 18:Y:36:ILE:HD11   | 1.00                     | 1.00              |
| 22:b:6010:CLA:H162 | 22:b:6010:CLA:H112 | 1.32                     | 1.00              |
| 3:C:265:ILE:HD11   | 3:C:452:ALA:CB     | 1.91                     | 1.00              |
| 25:D:1050:BCR:HC8  | 25:D:1050:BCR:C33  | 1.91                     | 1.00              |
| 12:M:9:ILE:HD12    | 12:m:5009:ILE:HD11 | 1.44                     | 1.00              |
| 26:a:6063:LHG:H161 | 26:a:6063:LHG:H122 | 1.42                     | 1.00              |
| 3:c:5350:ILE:HG21  | 3:c:5359:TRP:HB2   | 1.43                     | 1.00              |
| 23:d:6039:PHO:CMA  | 23:d:6039:PHO:CBA  | 2.30                     | 1.00              |
| 22:B:1010:CLA:HBD  | 22:B:1010:CLA:C1   | 1.92                     | 1.00              |
| 22:B:1011:CLA:H193 | 22:H:1017:CLA:H101 | 1.00                     | 1.00              |
| 22:B:1015:CLA:CAD  | 22:B:1015:CLA:CED  | 2.40                     | 1.00              |
| 25:B:1047:BCR:C24  | 25:t:1046:BCR:H353 | 1.92                     | 1.00              |
| 3:C:166:ILE:HD12   | 3:C:249:ILE:HD12   | 1.44                     | 1.00              |
| 22:C:1031:CLA:HMA2 | 22:C:1031:CLA:O2A  | 1.62                     | 1.00              |
| 4:D:91:LEU:HA      | 22:D:1008:CLA:CED  | 1.92                     | 1.00              |
| 16:V:45:ILE:H      | 16:V:45:ILE:HD12   | 1.22                     | 0.99              |
| 1:a:5060:ILE:HD11  | 1:a:5083:VAL:HB    | 1.41                     | 0.99              |
| 16:V:118:HIS:HD2   | 16:V:119:PRO:HD2   | 1.23                     | 0.99              |
| 22:b:6023:CLA:CED  | 22:b:6024:CLA:CBB  | 2.40                     | 0.99              |
| 3:c:5167:VAL:HG12  | 3:c:5168:LEU:HD12  | 1.44                     | 0.99              |
| 3:c:5417:VAL:HG11  | 16:v:5068:VAL:HG11 | 1.40                     | 0.99              |
| 2:B:59:GLY:HA3     | 2:B:329:PRO:HB3    | 1.45                     | 0.99              |
| 3:C:49:LEU:HB3     | 3:C:133:ALA:HA     | 1.40                     | 0.99              |
| 3:c:5166:ILE:HD12  | 3:c:5249:ILE:HD12  | 1.44                     | 0.99              |
| 16:v:5045:ILE:HD12 | 16:v:5045:ILE:H    | 1.23                     | 0.99              |
| 1:A:223:LEU:O      | 1:A:224:ILE:HB     | 1.60                     | 0.99              |
| 22:A:1003:CLA:HED2 | 22:A:1003:CLA:HAA2 | 1.01                     | 0.99              |
| 22:C:1025:CLA:CHB  | 22:C:1025:CLA:C1   | 2.41                     | 0.99              |
| 25:C:1052:BCR:C37  | 25:C:1052:BCR:H383 | 1.90                     | 0.99              |
| 25:T:6046:BCR:H353 | 25:b:6047:BCR:C24  | 1.92                     | 0.99              |
| 22:c:6025:CLA:CHB  | 22:c:6025:CLA:C1   | 2.41                     | 0.99              |
| 22:c:6030:CLA:HBB2 | 22:c:6031:CLA:HED1 | 1.45                     | 0.99              |
| 2:B:149:LEU:CG     | 22:B:1011:CLA:HBC1 | 1.92                     | 0.99              |
| 12:M:29:THR:O      | 12:M:32:GLN:HG2    | 1.61                     | 0.99              |
| 22:b:6012:CLA:C3B  | 22:b:6015:CLA:HBB2 | 1.91                     | 0.99              |
| 22:b:6012:CLA:CGA  | 22:b:6020:CLA:H141 | 1.91                     | 0.99              |
| 4:d:5037:LEU:HD22  | 4:d:5128:ARG:HD3   | 1.41                     | 0.99              |
| 22:B:1012:CLA:CGA  | 22:B:1020:CLA:H141 | 1.91                     | 0.99              |
| 22:C:1033:CLA:CMA  | 22:K:1034:CLA:C3C  | 2.41                     | 0.99              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:d:6005:CLA:HBC2 | 22:d:6004:CLA:HBB2 | 1.42                     | 0.99              |
| 16:v:5118:HIS:HD2  | 16:v:5119:PRO:HD2  | 1.23                     | 0.99              |
| 2:B:278:SER:HB3    | 2:B:281:GLN:HG2    | 1.41                     | 0.99              |
| 29:C:1056:DGD:HE5  | 29:C:1056:DGD:HD62 | 0.99                     | 0.99              |
| 3:c:5343:ARG:NH1   | 3:c:5348:GLU:CG    | 2.21                     | 0.99              |
| 28:d:6059:MGE:H211 | 28:d:6059:MGE:CFB  | 1.92                     | 0.99              |
| 2:B:341:LYS:HB3    | 2:B:406:LEU:HD22   | 1.45                     | 0.99              |
| 22:B:1012:CLA:C3B  | 22:B:1015:CLA:HBB2 | 1.91                     | 0.99              |
| 4:D:91:LEU:HA      | 22:D:1008:CLA:HED1 | 1.41                     | 0.99              |
| 22:b:6010:CLA:HBD  | 22:b:6010:CLA:C1   | 1.92                     | 0.99              |
| 2:B:75:TRP:NE1     | 2:B:94:GLU:HB2     | 1.76                     | 0.99              |
| 22:B:1009:CLA:H142 | 22:B:1009:CLA:C10  | 1.89                     | 0.99              |
| 22:B:1015:CLA:H41  | 22:B:1015:CLA:H72  | 1.41                     | 0.99              |
| 16:V:34:LEU:HD22   | 16:V:47:LEU:HB3    | 1.44                     | 0.99              |
| 22:b:6009:CLA:HMB3 | 25:h:6049:BCR:H271 | 1.01                     | 0.99              |
| 3:c:5229:ASN:HD22  | 3:c:5229:ASN:H     | 1.03                     | 0.99              |
| 22:c:6033:CLA:CMA  | 22:k:6034:CLA:C3C  | 2.41                     | 0.99              |
| 4:d:5265:ARG:HG3   | 4:d:5265:ARG:HH11  | 1.23                     | 0.99              |
| 14:t:5018:PHE:HA   | 25:t:1046:BCR:H332 | 1.45                     | 0.99              |
| 23:D:1039:PHO:CMA  | 22:D:1004:CLA:C14  | 2.41                     | 0.98              |
| 2:b:5065:PHE:HE2   | 22:b:6012:CLA:HMA2 | 1.23                     | 0.98              |
| 22:b:6015:CLA:CAD  | 22:b:6015:CLA:CED  | 2.40                     | 0.98              |
| 22:c:6030:CLA:C3D  | 22:c:6030:CLA:HED2 | 1.93                     | 0.98              |
| 25:d:6050:BCR:HC8  | 25:d:6050:BCR:H331 | 1.43                     | 0.98              |
| 16:v:5038:LEU:HA   | 16:v:5095:ILE:HG22 | 1.45                     | 0.98              |
| 1:A:269:ARG:HD3    | 4:D:222:LEU:HD11   | 1.45                     | 0.98              |
| 2:B:324:LEU:HA     | 4:D:293:LEU:HD22   | 1.43                     | 0.98              |
| 3:c:5042:LEU:HD21  | 3:c:5048:LYS:HG2   | 1.45                     | 0.98              |
| 2:b:5475:PHE:CD1   | 4:d:5140:PRO:CG    | 2.45                     | 0.98              |
| 22:b:6021:CLA:H142 | 22:b:6021:CLA:H102 | 0.99                     | 0.98              |
| 22:C:1025:CLA:H42  | 22:C:1025:CLA:C2B  | 1.93                     | 0.98              |
| 22:c:6025:CLA:H151 | 22:c:6031:CLA:H92  | 1.34                     | 0.98              |
| 22:c:6033:CLA:H171 | 22:c:6033:CLA:C14  | 1.92                     | 0.98              |
| 28:l:6061:MGE:H1G2 | 28:l:6061:MGE:O1B  | 1.63                     | 0.98              |
| 1:A:156:ALA:HA     | 1:A:160:ILE:HD12   | 1.43                     | 0.98              |
| 23:A:1038:PHO:HMB3 | 22:D:1005:CLA:H52  | 1.46                     | 0.98              |
| 3:C:417:VAL:HG11   | 16:V:68:VAL:HG11   | 1.40                     | 0.98              |
| 22:C:1026:CLA:HBA1 | 22:C:1027:CLA:HAC1 | 0.98                     | 0.98              |
| 1:a:5156:ALA:HA    | 1:a:5160:ILE:HD12  | 1.43                     | 0.98              |
| 22:b:6019:CLA:H93  | 28:l:6061:MGE:H9A2 | 1.41                     | 0.98              |
| 3:c:5091:HIS:CD2   | 22:c:6026:CLA:HED1 | 1.97                     | 0.98              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6031:CLA:HMA2 | 22:c:6031:CLA:O2A  | 1.62                     | 0.98              |
| 14:t:5004:ILE:HD13 | 14:t:5005:THR:N    | 1.78                     | 0.98              |
| 3:C:91:HIS:CD2     | 22:C:1026:CLA:HED1 | 1.97                     | 0.98              |
| 14:T:4:ILE:HD13    | 14:T:5:THR:N       | 1.78                     | 0.98              |
| 22:b:6011:CLA:H193 | 22:h:6017:CLA:H101 | 1.00                     | 0.98              |
| 22:c:6029:CLA:C4C  | 22:c:6029:CLA:C4   | 2.42                     | 0.98              |
| 1:A:279:ARG:CD     | 4:D:208:ALA:HB1    | 1.93                     | 0.98              |
| 22:B:1010:CLA:H162 | 22:B:1010:CLA:H112 | 1.31                     | 0.98              |
| 22:B:1010:CLA:C11  | 22:B:1010:CLA:C16  | 2.30                     | 0.98              |
| 22:B:1023:CLA:CED  | 22:B:1024:CLA:CBB  | 2.40                     | 0.98              |
| 22:C:1030:CLA:HED2 | 22:C:1030:CLA:C3D  | 1.93                     | 0.98              |
| 1:a:5159:LEU:HD21  | 29:c:6055:DGD:HA71 | 1.45                     | 0.98              |
| 2:b:5278:SER:HB3   | 2:b:5281:GLN:HG2   | 1.41                     | 0.98              |
| 22:b:6021:CLA:OBD  | 22:b:6022:CLA:HHC  | 1.59                     | 0.98              |
| 2:B:475:PHE:CD1    | 4:D:140:PRO:CG     | 2.45                     | 0.98              |
| 3:C:348:GLU:HB3    | 13:O:42:ALA:HB1    | 1.43                     | 0.98              |
| 28:D:1059:MGE:H211 | 28:D:1059:MGE:CFB  | 1.92                     | 0.98              |
| 22:c:6033:CLA:HED3 | 22:c:6033:CLA:OBD  | 1.62                     | 0.98              |
| 10:k:5032:PHE:CD1  | 25:k:6052:BCR:H383 | 1.98                     | 0.98              |
| 22:C:1025:CLA:H151 | 22:C:1031:CLA:H92  | 1.34                     | 0.98              |
| 22:C:1027:CLA:H152 | 25:Z:1053:BCR:H332 | 1.42                     | 0.98              |
| 1:a:5223:LEU:O     | 1:a:5224:ILE:HB    | 1.60                     | 0.98              |
| 2:B:105:GLY:CA     | 25:B:1047:BCR:C40  | 2.42                     | 0.98              |
| 1:a:5228:THR:HG22  | 1:a:5229:GLU:H     | 1.27                     | 0.98              |
| 3:c:5271:TYR:CE1   | 22:c:6031:CLA:HAC1 | 1.99                     | 0.98              |
| 22:D:1008:CLA:H141 | 22:D:1008:CLA:H172 | 1.46                     | 0.97              |
| 2:b:5105:GLY:CA    | 25:b:6047:BCR:C40  | 2.42                     | 0.97              |
| 22:b:6010:CLA:C11  | 22:b:6010:CLA:C16  | 2.30                     | 0.97              |
| 22:b:6012:CLA:HMB1 | 22:b:6015:CLA:HBB1 | 1.46                     | 0.97              |
| 24:A:1043:PQ9:C45  | 28:D:1059:MGE:H101 | 1.94                     | 0.97              |
| 22:C:1033:CLA:OBD  | 22:C:1033:CLA:HED3 | 1.62                     | 0.97              |
| 1:a:5054:ALA:HB2   | 1:a:5072:LEU:HD12  | 1.42                     | 0.97              |
| 22:A:1003:CLA:HED2 | 22:A:1003:CLA:H2A  | 1.41                     | 0.97              |
| 23:d:6039:PHO:CMA  | 22:d:6004:CLA:C14  | 2.41                     | 0.97              |
| 24:d:6042:PQ9:H242 | 28:l:6061:MGE:H212 | 1.46                     | 0.97              |
| 25:z:6053:BCR:H23C | 25:z:6053:BCR:C38  | 1.90                     | 0.97              |
| 2:B:220:ARG:HD3    | 2:B:221:PRO:HD2    | 1.43                     | 0.97              |
| 22:D:1005:CLA:HBC2 | 22:D:1004:CLA:HBB2 | 1.42                     | 0.97              |
| 4:d:5091:LEU:HA    | 22:d:6008:CLA:CED  | 1.92                     | 0.97              |
| 22:C:1029:CLA:C4C  | 22:C:1029:CLA:C4   | 2.42                     | 0.97              |
| 22:B:1014:CLA:HBA1 | 22:B:1014:CLA:CHA  | 1.95                     | 0.97              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1016:CLA:H52  | 22:H:1017:CLA:H91  | 0.97                     | 0.97              |
| 3:c:5348:GLU:HB3   | 13:o:5042:ALA:HB1  | 1.43                     | 0.97              |
| 16:v:5034:LEU:HD22 | 16:v:5047:LEU:HB3  | 1.44                     | 0.97              |
| 22:B:1021:CLA:H142 | 22:B:1021:CLA:H102 | 0.99                     | 0.97              |
| 3:C:271:TYR:CE1    | 22:C:1031:CLA:HAC1 | 1.99                     | 0.97              |
| 23:D:1039:PHO:CBA  | 23:D:1039:PHO:HMA1 | 1.94                     | 0.97              |
| 22:D:1008:CLA:H141 | 22:D:1008:CLA:C17  | 1.95                     | 0.97              |
| 2:b:5059:GLY:HA3   | 2:b:5329:PRO:HB3   | 1.45                     | 0.97              |
| 22:b:6015:CLA:H41  | 22:b:6015:CLA:H72  | 1.41                     | 0.97              |
| 22:c:6027:CLA:C17  | 22:c:6027:CLA:H121 | 1.91                     | 0.97              |
| 22:c:6033:CLA:HED3 | 22:c:6033:CLA:CAD  | 1.95                     | 0.97              |
| 25:d:6050:BCR:HC8  | 25:d:6050:BCR:C33  | 1.91                     | 0.97              |
| 1:A:159:LEU:HD21   | 29:C:1055:DGD:HA71 | 1.45                     | 0.97              |
| 1:A:228:THR:HG22   | 1:A:229:GLU:H      | 1.27                     | 0.97              |
| 3:C:50:LEU:C       | 3:C:50:LEU:CD2     | 2.30                     | 0.97              |
| 7:H:6:TRP:CD1      | 7:H:10:ILE:HD11    | 1.99                     | 0.97              |
| 2:b:5220:ARG:HD3   | 2:b:5221:PRO:HD2   | 1.43                     | 0.97              |
| 22:b:6020:CLA:C10  | 22:b:6020:CLA:C16  | 2.43                     | 0.97              |
| 22:B:1011:CLA:CAD  | 22:B:1013:CLA:H12  | 1.95                     | 0.97              |
| 22:B:1012:CLA:HMB1 | 22:B:1015:CLA:HBB1 | 1.46                     | 0.97              |
| 22:C:1032:CLA:H151 | 10:K:33:PHE:HZ     | 0.81                     | 0.97              |
| 22:C:1033:CLA:HED3 | 22:C:1033:CLA:CAD  | 1.94                     | 0.97              |
| 25:b:6047:BCR:C39  | 25:b:6047:BCR:C37  | 2.30                     | 0.97              |
| 22:c:6026:CLA:HBA1 | 22:c:6027:CLA:HAC1 | 0.98                     | 0.97              |
| 4:d:5160:TYR:OH    | 27:d:6068:IOD:I    | 2.51                     | 0.97              |
| 7:h:5006:TRP:CD1   | 7:h:5010:ILE:HD11  | 1.99                     | 0.97              |
| 25:k:6051:BCR:H403 | 25:k:6051:BCR:C23  | 1.94                     | 0.97              |
| 25:B:1048:BCR:C40  | 25:B:1048:BCR:C37  | 2.30                     | 0.97              |
| 22:C:1032:CLA:CAB  | 22:K:1034:CLA:HMC3 | 1.95                     | 0.97              |
| 22:C:1033:CLA:H171 | 22:C:1033:CLA:C14  | 1.92                     | 0.97              |
| 22:b:6011:CLA:CAD  | 22:b:6013:CLA:H12  | 1.95                     | 0.97              |
| 23:d:6039:PHO:CBA  | 23:d:6039:PHO:HMA1 | 1.94                     | 0.97              |
| 23:A:1038:PHO:H93  | 22:D:1005:CLA:H18  | 1.46                     | 0.96              |
| 22:B:1009:CLA:C1A  | 22:B:1009:CLA:CGA  | 2.43                     | 0.96              |
| 22:B:1020:CLA:C10  | 22:B:1020:CLA:C16  | 2.43                     | 0.96              |
| 22:B:1022:CLA:H91  | 22:B:1022:CLA:C12  | 1.92                     | 0.96              |
| 25:D:1050:BCR:H372 | 28:D:1059:MGE:C3A  | 1.95                     | 0.96              |
| 1:a:5269:ARG:HD3   | 4:d:5222:LEU:HD11  | 1.45                     | 0.96              |
| 22:b:6011:CLA:HED2 | 22:b:6012:CLA:HED3 | 1.46                     | 0.96              |
| 22:c:6032:CLA:CAB  | 22:k:6034:CLA:HMC3 | 1.95                     | 0.96              |
| 29:c:6056:DGD:HE5  | 29:c:6056:DGD:HD62 | 0.99                     | 0.96              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1023:CLA:CED  | 22:B:1024:CLA:HBB1 | 1.94                     | 0.96              |
| 1:a:5196:PRO:HB2   | 29:c:6057:DGD:HA81 | 1.47                     | 0.96              |
| 22:a:6003:CLA:HED2 | 22:a:6003:CLA:H2A  | 1.41                     | 0.96              |
| 22:b:6009:CLA:CGA  | 22:b:6009:CLA:C1A  | 2.43                     | 0.96              |
| 22:b:6014:CLA:C7   | 22:b:6014:CLA:C4   | 2.36                     | 0.96              |
| 22:C:1030:CLA:HBB2 | 22:C:1031:CLA:HED1 | 1.45                     | 0.96              |
| 22:C:1033:CLA:H143 | 22:C:1033:CLA:C17  | 1.95                     | 0.96              |
| 25:D:1050:BCR:HC8  | 25:D:1050:BCR:H331 | 1.43                     | 0.96              |
| 25:d:6050:BCR:H372 | 28:d:6059:MGE:C3A  | 1.95                     | 0.96              |
| 24:a:6043:PQ9:C45  | 28:d:6059:MGE:H101 | 1.94                     | 0.96              |
| 22:b:6022:CLA:H143 | 22:b:6022:CLA:C8   | 1.95                     | 0.96              |
| 22:d:6008:CLA:H141 | 22:d:6008:CLA:H172 | 1.46                     | 0.96              |
| 2:B:174:LEU:HD13   | 2:B:174:LEU:N      | 1.79                     | 0.96              |
| 3:c:5049:LEU:CD2   | 22:c:6035:CLA:HMA3 | 1.94                     | 0.96              |
| 22:d:6008:CLA:H141 | 22:d:6008:CLA:C17  | 1.95                     | 0.96              |
| 1:A:212:CYS:HB2    | 4:D:211:CYS:HB2    | 1.43                     | 0.96              |
| 1:a:5339:PHE:HB3   | 1:a:5340:PRO:HD2   | 1.47                     | 0.96              |
| 2:B:103:LEU:HB2    | 22:B:1014:CLA:H92  | 1.45                     | 0.96              |
| 22:C:1029:CLA:C5   | 22:C:1029:CLA:CHC  | 2.43                     | 0.96              |
| 28:L:1061:MGE:H1G2 | 28:L:1061:MGE:O1B  | 1.63                     | 0.96              |
| 16:V:38:LEU:HA     | 16:V:95:ILE:HG22   | 1.45                     | 0.96              |
| 22:b:6011:CLA:H2   | 22:b:6013:CLA:C9   | 1.95                     | 0.96              |
| 3:c:5042:LEU:HD11  | 3:c:5049:LEU:CD1   | 1.94                     | 0.96              |
| 22:c:6028:CLA:H2   | 29:c:6056:DGD:O1A  | 1.66                     | 0.96              |
| 22:c:6033:CLA:H143 | 22:c:6033:CLA:C17  | 1.95                     | 0.96              |
| 22:C:1029:CLA:HMA2 | 22:C:1029:CLA:HBA2 | 1.48                     | 0.96              |
| 24:D:1042:PQ9:C24  | 28:L:1061:MGE:H263 | 1.95                     | 0.96              |
| 1:a:5205:VAL:HB    | 1:a:5279:ARG:NH1   | 1.81                     | 0.96              |
| 22:a:6003:CLA:HED2 | 22:a:6003:CLA:HAA2 | 1.01                     | 0.96              |
| 22:a:6003:CLA:H41  | 22:a:6003:CLA:C7   | 1.91                     | 0.96              |
| 22:b:6011:CLA:H2   | 22:b:6013:CLA:H92  | 1.46                     | 0.96              |
| 22:b:6012:CLA:HBB1 | 22:b:6015:CLA:HBB2 | 1.46                     | 0.96              |
| 3:c:5348:GLU:HB3   | 13:o:5042:ALA:CB   | 1.95                     | 0.96              |
| 22:c:6029:CLA:H52  | 22:c:6029:CLA:CHC  | 1.96                     | 0.96              |
| 22:B:1022:CLA:C8   | 22:B:1022:CLA:H143 | 1.95                     | 0.96              |
| 3:C:49:LEU:CD2     | 3:C:52:ALA:N       | 2.28                     | 0.96              |
| 3:C:350:ILE:HG21   | 3:C:359:TRP:HB2    | 1.43                     | 0.96              |
| 22:C:1029:CLA:CHC  | 22:C:1029:CLA:H52  | 1.96                     | 0.96              |
| 25:K:1051:BCR:H403 | 25:K:1051:BCR:C23  | 1.94                     | 0.96              |
| 12:M:9:ILE:HD11    | 12:m:5009:ILE:HD12 | 1.47                     | 0.96              |
| 25:Z:1053:BCR:H23C | 25:Z:1053:BCR:C38  | 1.91                     | 0.96              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:a:6038:PHO:HMB3 | 22:d:6005:CLA:H52  | 1.46                     | 0.96              |
| 24:d:6042:PQ9:C24  | 28:l:6061:MGE:H263 | 1.95                     | 0.96              |
| 22:B:1022:CLA:H143 | 22:B:1022:CLA:C7   | 1.96                     | 0.95              |
| 2:b:5169:SER:HB3   | 2:b:5176:GLY:CA    | 1.96                     | 0.95              |
| 5:e:5008:ARG:NE    | 6:f:5013:TYR:HB2   | 1.82                     | 0.95              |
| 22:B:1011:CLA:H2   | 22:B:1013:CLA:C9   | 1.95                     | 0.95              |
| 22:B:1023:CLA:H91  | 22:B:1024:CLA:H151 | 1.47                     | 0.95              |
| 29:C:1057:DGD:CEA  | 28:D:1059:MGE:H222 | 1.96                     | 0.95              |
| 23:a:6038:PHO:H93  | 22:d:6005:CLA:H18  | 1.46                     | 0.95              |
| 4:d:5188:PHE:CE2   | 4:d:5326:ARG:HG2   | 2.01                     | 0.95              |
| 22:B:1011:CLA:HED2 | 22:B:1012:CLA:HED1 | 0.96                     | 0.95              |
| 22:b:6016:CLA:HBC3 | 22:b:6016:CLA:HHD  | 1.49                     | 0.95              |
| 22:b:6023:CLA:CED  | 22:b:6024:CLA:HBB1 | 1.94                     | 0.95              |
| 22:c:6026:CLA:H122 | 22:c:6026:CLA:C7   | 1.95                     | 0.95              |
| 22:c:6029:CLA:CHC  | 22:c:6029:CLA:C5   | 2.43                     | 0.95              |
| 22:c:6035:CLA:HBB2 | 22:k:6034:CLA:HMA2 | 1.48                     | 0.95              |
| 22:B:1020:CLA:H161 | 22:B:1020:CLA:H101 | 1.47                     | 0.95              |
| 3:C:155:ASN:HA     | 3:C:158:THR:HG22   | 1.49                     | 0.95              |
| 25:Z:1053:BCR:H383 | 25:Z:1053:BCR:C23  | 1.97                     | 0.95              |
| 2:b:5008:VAL:O     | 2:b:5011:VAL:HG23  | 1.67                     | 0.95              |
| 2:b:5103:LEU:HB2   | 22:b:6014:CLA:H92  | 1.44                     | 0.95              |
| 22:b:6015:CLA:C7   | 22:b:6015:CLA:C4   | 2.41                     | 0.95              |
| 22:b:6022:CLA:H143 | 22:b:6022:CLA:C10  | 1.97                     | 0.95              |
| 22:c:6025:CLA:C12  | 25:c:6054:BCR:H351 | 1.96                     | 0.95              |
| 29:c:6057:DGD:CEA  | 28:d:6059:MGE:H222 | 1.96                     | 0.95              |
| 22:C:1025:CLA:C12  | 25:C:1054:BCR:H351 | 1.96                     | 0.95              |
| 22:a:6006:CLA:H161 | 24:a:6043:PQ9:H443 | 1.48                     | 0.95              |
| 28:b:6060:MGE:H8A2 | 11:l:5023:LEU:HD21 | 1.47                     | 0.95              |
| 22:c:6030:CLA:H143 | 22:c:6030:CLA:H171 | 1.47                     | 0.95              |
| 16:v:5148:GLU:HA   | 16:v:5151:ILE:HD11 | 1.48                     | 0.95              |
| 22:A:1003:CLA:HHD  | 22:A:1003:CLA:HBC2 | 1.47                     | 0.95              |
| 3:C:46:SER:OG      | 3:C:149:TYR:HB3    | 1.65                     | 0.95              |
| 3:C:348:GLU:HB3    | 13:O:42:ALA:CB     | 1.95                     | 0.95              |
| 22:C:1030:CLA:H143 | 22:C:1030:CLA:H171 | 1.48                     | 0.95              |
| 29:C:1055:DGD:CIB  | 29:C:1055:DGD:HBF1 | 1.97                     | 0.95              |
| 2:B:169:SER:HB3    | 2:B:176:GLY:CA     | 1.96                     | 0.95              |
| 4:D:188:PHE:CE2    | 4:D:326:ARG:HG2    | 2.01                     | 0.95              |
| 22:B:1021:CLA:HED3 | 22:B:1021:CLA:H2A  | 0.94                     | 0.94              |
| 3:c:5046:SER:OG    | 3:c:5149:TYR:HB3   | 1.65                     | 0.94              |
| 25:c:6054:BCR:C40  | 25:c:6054:BCR:C23  | 2.30                     | 0.94              |
| 4:d:5148:ALA:HB3   | 4:d:5149:PRO:HD3   | 1.48                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1011:CLA:H2   | 22:B:1013:CLA:H92  | 1.46                     | 0.94              |
| 22:B:1018:CLA:H102 | 22:B:1023:CLA:CAA  | 1.97                     | 0.94              |
| 22:B:1022:CLA:H143 | 22:B:1022:CLA:C10  | 1.97                     | 0.94              |
| 3:C:264:PHE:N      | 3:C:264:PHE:CD2    | 2.30                     | 0.94              |
| 1:a:5205:VAL:CA    | 1:a:5279:ARG:NH1   | 2.28                     | 0.94              |
| 2:b:5341:LYS:HB3   | 2:b:5406:LEU:HD22  | 1.45                     | 0.94              |
| 22:b:6022:CLA:H143 | 22:b:6022:CLA:C7   | 1.96                     | 0.94              |
| 22:B:1015:CLA:C7   | 22:B:1015:CLA:C4   | 2.41                     | 0.94              |
| 22:C:1035:CLA:C2B  | 25:C:1052:BCR:H271 | 1.97                     | 0.94              |
| 22:b:6011:CLA:H193 | 22:h:6017:CLA:C10  | 1.95                     | 0.94              |
| 22:c:6025:CLA:H42  | 22:c:6025:CLA:C2B  | 1.93                     | 0.94              |
| 25:h:6049:BCR:C39  | 25:h:6049:BCR:C23  | 2.30                     | 0.94              |
| 10:k:5032:PHE:CZ   | 25:k:6052:BCR:H361 | 2.02                     | 0.94              |
| 3:C:263:ALA:CB     | 3:C:264:PHE:CE2    | 2.51                     | 0.94              |
| 13:O:80:GLU:O      | 13:O:82:PRO:HD3    | 1.68                     | 0.94              |
| 22:b:6011:CLA:C3D  | 22:b:6013:CLA:H12  | 1.96                     | 0.94              |
| 22:B:1011:CLA:HED2 | 22:B:1012:CLA:HED3 | 1.46                     | 0.94              |
| 7:H:12:ARG:HH12    | 7:H:15:ASN:HB3     | 1.30                     | 0.94              |
| 1:a:5187:GLN:HG3   | 1:a:5325:ASN:HD21  | 1.32                     | 0.94              |
| 22:b:6014:CLA:CHA  | 22:b:6014:CLA:HBA1 | 1.95                     | 0.94              |
| 22:b:6023:CLA:H91  | 22:b:6024:CLA:H151 | 1.47                     | 0.94              |
| 9:j:5021:VAL:HG12  | 9:j:5022:ILE:HD12  | 1.48                     | 0.94              |
| 22:B:1012:CLA:HBB1 | 22:B:1015:CLA:HBB2 | 1.46                     | 0.94              |
| 5:E:8:ARG:NE       | 6:F:13:TYR:HB2     | 1.81                     | 0.94              |
| 14:T:23:PHE:HZ     | 2:b:5112:CYS:SG    | 1.89                     | 0.94              |
| 25:d:6050:BCR:H23C | 25:d:6050:BCR:C38  | 1.90                     | 0.94              |
| 7:h:5012:ARG:HH12  | 7:h:5015:ASN:HB3   | 1.30                     | 0.94              |
| 22:A:1006:CLA:H161 | 24:A:1043:PQ9:H443 | 1.47                     | 0.94              |
| 2:B:8:VAL:O        | 2:B:11:VAL:HG23    | 1.67                     | 0.94              |
| 22:b:6020:CLA:H161 | 22:b:6020:CLA:H101 | 1.47                     | 0.94              |
| 3:c:5224:ILE:HG23  | 25:c:6054:BCR:H381 | 1.47                     | 0.94              |
| 22:c:6033:CLA:HHC  | 22:c:6033:CLA:HBB1 | 1.49                     | 0.94              |
| 29:c:6056:DGD:HD61 | 29:c:6056:DGD:HE3  | 0.94                     | 0.94              |
| 13:o:5080:GLU:O    | 13:o:5082:PRO:HD3  | 1.68                     | 0.94              |
| 22:B:1018:CLA:H102 | 22:B:1023:CLA:HAA1 | 1.50                     | 0.94              |
| 22:C:1026:CLA:H122 | 22:C:1026:CLA:C7   | 1.95                     | 0.94              |
| 22:C:1029:CLA:NC   | 22:C:1029:CLA:C4   | 2.30                     | 0.94              |
| 22:C:1029:CLA:H11  | 22:C:1029:CLA:C4D  | 1.98                     | 0.94              |
| 22:D:1008:CLA:H193 | 22:D:1008:CLA:H143 | 1.33                     | 0.94              |
| 25:D:1050:BCR:H23C | 25:D:1050:BCR:C38  | 1.91                     | 0.94              |
| 14:T:18:PHE:HA     | 25:T:6046:BCR:C33  | 1.96                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:T:6046:BCR:HC8  | 25:T:6046:BCR:C33  | 1.96                     | 0.94              |
| 25:T:6048:BCR:H371 | 25:T:6048:BCR:H403 | 1.33                     | 0.94              |
| 22:b:6016:CLA:H52  | 22:h:6017:CLA:H91  | 0.97                     | 0.94              |
| 3:c:5179:ALA:HB1   | 3:c:5199:ILE:HD13  | 1.49                     | 0.94              |
| 22:c:6029:CLA:HBA2 | 22:c:6029:CLA:HMA2 | 1.48                     | 0.94              |
| 22:c:6031:CLA:HHD  | 22:c:6031:CLA:CBC  | 1.98                     | 0.94              |
| 29:c:6055:DGD:HB1  | 29:c:6055:DGD:CIB  | 1.97                     | 0.94              |
| 4:D:261:PHE:H      | 24:D:1042:PQ9:H91  | 1.32                     | 0.94              |
| 31:F:1040:HEM:HMA1 | 31:F:1040:HEM:CBA  | 1.97                     | 0.94              |
| 22:b:6023:CLA:H13  | 22:b:6024:CLA:HMA1 | 1.50                     | 0.94              |
| 3:c:5263:ALA:HB3   | 3:c:5264:PHE:CD2   | 2.03                     | 0.94              |
| 22:c:6035:CLA:C2B  | 25:k:6052:BCR:H271 | 1.97                     | 0.94              |
| 1:A:183:MET:HB3    | 22:A:1003:CLA:HBC3 | 1.48                     | 0.94              |
| 26:A:1063:LHG:H321 | 22:K:1034:CLA:H151 | 1.50                     | 0.94              |
| 3:C:333:GLY:H      | 3:C:338:GLY:HA2    | 1.33                     | 0.94              |
| 10:K:33:PHE:O      | 10:K:33:PHE:HD2    | 1.51                     | 0.94              |
| 22:b:6022:CLA:H92  | 22:b:6022:CLA:CBC  | 1.98                     | 0.94              |
| 3:c:5155:ASN:HA    | 3:c:5158:THR:HG22  | 1.49                     | 0.94              |
| 4:d:5261:PHE:H     | 24:d:6042:PQ9:H91  | 1.32                     | 0.94              |
| 25:t:1046:BCR:HC8  | 25:t:1046:BCR:C33  | 1.96                     | 0.94              |
| 3:C:117:VAL:HG11   | 22:C:1027:CLA:H42  | 1.50                     | 0.93              |
| 3:C:179:ALA:HB1    | 3:C:199:ILE:HD13   | 1.49                     | 0.93              |
| 3:C:263:ALA:HB3    | 3:C:264:PHE:CD2    | 2.03                     | 0.93              |
| 22:a:6003:CLA:HBC2 | 22:a:6003:CLA:HHD  | 1.47                     | 0.93              |
| 23:a:6038:PHO:C20  | 22:d:6005:CLA:C2B  | 2.46                     | 0.93              |
| 22:b:6018:CLA:H102 | 22:b:6023:CLA:CAA  | 1.97                     | 0.93              |
| 22:b:6018:CLA:H102 | 22:b:6023:CLA:HAA1 | 1.50                     | 0.93              |
| 22:b:6021:CLA:HED3 | 22:b:6021:CLA:H2A  | 0.94                     | 0.93              |
| 22:d:6005:CLA:HBC1 | 22:d:6004:CLA:HBB2 | 1.48                     | 0.93              |
| 22:A:1003:CLA:H41  | 22:A:1003:CLA:C7   | 1.91                     | 0.93              |
| 22:B:1011:CLA:C3D  | 22:B:1013:CLA:H12  | 1.96                     | 0.93              |
| 3:C:224:ILE:HG23   | 25:C:1054:BCR:H381 | 1.47                     | 0.93              |
| 22:C:1033:CLA:HBB1 | 22:C:1033:CLA:HHC  | 1.49                     | 0.93              |
| 29:C:1056:DGD:HD61 | 29:C:1056:DGD:HE3  | 0.94                     | 0.93              |
| 25:D:1050:BCR:C22  | 28:D:1059:MGE:H3A1 | 1.97                     | 0.93              |
| 16:V:148:GLU:HA    | 16:V:151:ILE:HD11  | 1.48                     | 0.93              |
| 3:c:5333:GLY:H     | 3:c:5338:GLY:HA2   | 1.33                     | 0.93              |
| 25:d:6050:BCR:C22  | 28:d:6059:MGE:H3A1 | 1.98                     | 0.93              |
| 22:B:1022:CLA:H92  | 22:B:1022:CLA:CBC  | 1.98                     | 0.93              |
| 22:C:1025:CLA:H152 | 22:C:1031:CLA:H92  | 1.49                     | 0.93              |
| 1:a:5183:MET:HB3   | 22:a:6003:CLA:HBC3 | 1.48                     | 0.93              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6015:CLA:CB   | 25:b:6045:BCR:C34  | 2.45                     | 0.93              |
| 25:z:6053:BCR:H383 | 25:z:6053:BCR:C23  | 1.97                     | 0.93              |
| 1:A:187:GLN:HG3    | 1:A:325:ASN:HD21   | 1.32                     | 0.93              |
| 22:B:1022:CLA:H93  | 22:B:1022:CLA:H142 | 0.95                     | 0.93              |
| 22:C:1028:CLA:H2   | 29:C:1056:DGD:O1A  | 1.66                     | 0.93              |
| 22:C:1029:CLA:CMD  | 22:C:1031:CLA:HAB  | 1.99                     | 0.93              |
| 25:B:1047:BCR:H371 | 25:B:1047:BCR:H392 | 1.32                     | 0.93              |
| 2:b:5311:PHE:HE2   | 2:b:5317:ASN:HD21  | 1.15                     | 0.93              |
| 2:b:5370:LEU:HB2   | 2:b:5379:ALA:HB3   | 1.47                     | 0.93              |
| 22:B:1016:CLA:H52  | 22:H:1017:CLA:H92  | 1.49                     | 0.93              |
| 22:B:1022:CLA:H42  | 22:B:1022:CLA:O1A  | 1.68                     | 0.93              |
| 23:D:1039:PHO:HMA3 | 22:D:1004:CLA:H102 | 1.50                     | 0.93              |
| 15:U:68:THR:HG22   | 15:U:71:GLN:H      | 1.33                     | 0.93              |
| 2:b:5174:LEU:HD13  | 2:b:5174:LEU:N     | 1.79                     | 0.93              |
| 22:c:6029:CLA:CMD  | 22:c:6031:CLA:HAB  | 1.99                     | 0.93              |
| 15:u:5068:THR:HG22 | 15:u:5071:GLN:H    | 1.33                     | 0.93              |
| 4:D:87:HIS:CD2     | 4:D:162:LEU:HA     | 2.04                     | 0.93              |
| 22:b:6011:CLA:HED2 | 22:b:6012:CLA:HED1 | 0.96                     | 0.93              |
| 22:c:6029:CLA:H11  | 22:c:6029:CLA:C4D  | 1.98                     | 0.93              |
| 29:C:1055:DGD:O2D  | 29:C:1055:DGD:HG31 | 1.67                     | 0.93              |
| 1:a:5142:TRP:HB3   | 3:c:5443:TRP:CH2   | 2.03                     | 0.93              |
| 22:b:6022:CLA:H93  | 22:b:6022:CLA:H142 | 0.95                     | 0.93              |
| 3:c:5263:ALA:CB    | 3:c:5264:PHE:CE2   | 2.51                     | 0.93              |
| 23:d:6039:PHO:HBA2 | 23:d:6039:PHO:HMA1 | 1.47                     | 0.93              |
| 10:k:5032:PHE:CE1  | 25:k:6052:BCR:C21  | 2.50                     | 0.93              |
| 22:B:1011:CLA:H193 | 22:H:1017:CLA:C10  | 1.95                     | 0.93              |
| 22:B:1011:CLA:C1   | 22:B:1013:CLA:H93  | 1.99                     | 0.93              |
| 28:B:1060:MGE:H8A2 | 11:L:23:LEU:HD21   | 1.47                     | 0.93              |
| 4:D:148:ALA:HB3    | 4:D:149:PRO:HD3    | 1.48                     | 0.93              |
| 9:J:10:LEU:HD13    | 9:J:10:LEU:H       | 1.34                     | 0.93              |
| 10:K:39:VAL:HG23   | 18:Y:36:ILE:CD1    | 1.96                     | 0.93              |
| 1:a:5205:VAL:CB    | 1:a:5279:ARG:NH1   | 2.30                     | 0.93              |
| 22:B:1014:CLA:C7   | 22:B:1014:CLA:C4   | 2.36                     | 0.93              |
| 3:C:56:HIS:C       | 3:C:58:GLY:H       | 1.72                     | 0.93              |
| 29:C:1057:DGD:HB2  | 29:C:1057:DGD:HBG3 | 1.51                     | 0.93              |
| 9:J:21:VAL:HG12    | 9:J:22:ILE:HD12    | 1.48                     | 0.93              |
| 25:T:6046:BCR:H331 | 25:T:6046:BCR:C8   | 1.92                     | 0.93              |
| 22:a:6003:CLA:H42  | 23:a:6038:PHO:C3B  | 1.99                     | 0.93              |
| 29:c:6056:DGD:C3E  | 29:c:6056:DGD:C6D  | 2.46                     | 0.93              |
| 1:A:142:TRP:HB3    | 3:C:443:TRP:CH2    | 2.03                     | 0.92              |
| 1:A:196:PRO:HB2    | 29:C:1057:DGD:HA81 | 1.47                     | 0.92              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:A:1038:PHO:C20  | 22:D:1005:CLA:CMB  | 2.48                     | 0.92              |
| 22:B:1012:CLA:C1D  | 22:B:1020:CLA:C20  | 2.47                     | 0.92              |
| 1:a:5224:ILE:H     | 2:b:5482:ILE:HG23  | 1.34                     | 0.92              |
| 22:c:6028:CLA:NC   | 29:c:6056:DGD:HA31 | 1.84                     | 0.92              |
| 4:d:5087:HIS:CD2   | 4:d:5162:LEU:HA    | 2.04                     | 0.92              |
| 1:a:5310:LYS:HB2   | 16:v:5028:GLU:HB3  | 1.51                     | 0.92              |
| 22:a:6003:CLA:CAA  | 22:a:6003:CLA:CED  | 2.30                     | 0.92              |
| 22:b:6022:CLA:O1A  | 22:b:6022:CLA:H42  | 1.68                     | 0.92              |
| 2:B:370:LEU:HB2    | 2:B:379:ALA:HB3    | 1.47                     | 0.92              |
| 25:B:1045:BCR:H331 | 25:B:1045:BCR:C8   | 1.98                     | 0.92              |
| 22:C:1028:CLA:NC   | 29:C:1056:DGD:HA31 | 1.84                     | 0.92              |
| 24:D:1042:PQ9:H242 | 28:L:1061:MGE:H212 | 1.46                     | 0.92              |
| 22:a:6006:CLA:CBB  | 22:d:6004:CLA:H51  | 1.99                     | 0.92              |
| 22:c:6025:CLA:H152 | 22:c:6031:CLA:H92  | 1.49                     | 0.92              |
| 1:A:279:ARG:NH1    | 23:A:1038:PHO:CMC  | 2.22                     | 0.92              |
| 2:B:83:GLU:HG2     | 2:B:86:ILE:HD11    | 1.51                     | 0.92              |
| 23:D:1039:PHO:HMA2 | 22:D:1004:CLA:H143 | 1.50                     | 0.92              |
| 22:b:6009:CLA:CED  | 22:b:6009:CLA:H2A  | 2.00                     | 0.92              |
| 25:b:6045:BCR:H331 | 25:b:6045:BCR:C8   | 1.98                     | 0.92              |
| 22:A:1003:CLA:H42  | 23:A:1038:PHO:C3B  | 1.99                     | 0.92              |
| 22:B:1021:CLA:HED3 | 22:B:1021:CLA:O1A  | 1.70                     | 0.92              |
| 26:a:6063:LHG:C29  | 22:c:6032:CLA:H72  | 1.99                     | 0.92              |
| 2:b:5083:GLU:HG2   | 2:b:5086:ILE:HD11  | 1.51                     | 0.92              |
| 22:c:6029:CLA:NC   | 22:c:6029:CLA:C4   | 2.30                     | 0.92              |
| 22:A:1006:CLA:CBB  | 22:D:1004:CLA:H51  | 1.99                     | 0.92              |
| 22:a:6003:CLA:H42  | 23:a:6038:PHO:NB   | 1.85                     | 0.92              |
| 24:a:6043:PQ9:H452 | 28:d:6059:MGE:H8A2 | 1.51                     | 0.92              |
| 26:a:6063:LHG:H321 | 22:k:6034:CLA:H151 | 1.50                     | 0.92              |
| 16:v:5118:HIS:CD2  | 16:v:5119:PRO:HD2  | 2.05                     | 0.92              |
| 23:A:1038:PHO:C20  | 22:D:1005:CLA:C2B  | 2.46                     | 0.92              |
| 22:B:1016:CLA:H51  | 22:H:1017:CLA:H112 | 1.52                     | 0.92              |
| 22:B:1023:CLA:H161 | 22:B:1023:CLA:H101 | 1.51                     | 0.92              |
| 16:V:118:HIS:CD2   | 16:V:119:PRO:HD2   | 2.05                     | 0.92              |
| 25:b:6045:BCR:H372 | 25:b:6045:BCR:H361 | 1.50                     | 0.92              |
| 3:c:5167:VAL:HA    | 3:c:5170:ILE:HD12  | 1.50                     | 0.92              |
| 3:c:5167:VAL:O     | 3:c:5170:ILE:HB    | 1.69                     | 0.92              |
| 22:B:1021:CLA:H2   | 22:B:1021:CLA:HMA3 | 1.52                     | 0.92              |
| 3:C:167:VAL:HA     | 3:C:170:ILE:HD12   | 1.50                     | 0.92              |
| 4:D:139:ARG:HH12   | 4:D:265:ARG:HH21   | 1.15                     | 0.92              |
| 10:k:5033:PHE:HB2  | 22:k:6034:CLA:H3A  | 1.51                     | 0.92              |
| 18:y:5044:GLY:O    | 18:y:5045:ASN:HB3  | 1.70                     | 0.92              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:z:5020:VAL:O    | 20:z:5024:PRO:HD2  | 1.69                     | 0.92              |
| 24:A:1043:PQ9:H452 | 28:D:1059:MGE:H8A2 | 1.51                     | 0.92              |
| 25:B:1045:BCR:H372 | 25:B:1045:BCR:H361 | 1.50                     | 0.92              |
| 22:C:1031:CLA:HHD  | 22:C:1031:CLA:CBC  | 1.98                     | 0.92              |
| 25:a:6044:BCR:H371 | 25:a:6044:BCR:H392 | 1.30                     | 0.92              |
| 22:b:6012:CLA:C1D  | 22:b:6020:CLA:C20  | 2.47                     | 0.92              |
| 29:c:6057:DGD:HAF2 | 28:d:6059:MGE:CCB  | 1.99                     | 0.92              |
| 5:e:5013:ILE:HG12  | 31:f:6040:HEM:HBC2 | 1.52                     | 0.92              |
| 31:f:6040:HEM:HMA1 | 31:f:6040:HEM:CBA  | 1.97                     | 0.92              |
| 1:A:272:HIS:CD2    | 4:D:218:VAL:HG21   | 2.04                     | 0.92              |
| 22:B:1014:CLA:HHD  | 22:B:1014:CLA:CBC  | 2.00                     | 0.92              |
| 22:B:1021:CLA:H2A  | 22:B:1021:CLA:O1A  | 1.61                     | 0.92              |
| 3:C:49:LEU:HD21    | 22:C:1035:CLA:HMA1 | 1.52                     | 0.92              |
| 18:Y:44:GLY:O      | 18:Y:45:ASN:HB3    | 1.70                     | 0.92              |
| 29:c:6055:DGD:O2D  | 29:c:6055:DGD:HG31 | 1.67                     | 0.92              |
| 3:c:5036:TRP:CZ3   | 3:c:5037:ALA:HB2   | 2.06                     | 0.91              |
| 1:A:76:ASN:ND2     | 11:L:33:SER:HB3    | 1.85                     | 0.91              |
| 22:B:1015:CLA:CBC  | 25:B:1045:BCR:C34  | 2.45                     | 0.91              |
| 3:C:167:VAL:O      | 3:C:170:ILE:HB     | 1.69                     | 0.91              |
| 23:a:6038:PHO:C20  | 22:d:6005:CLA:CMB  | 2.47                     | 0.91              |
| 2:b:5174:LEU:CD2   | 2:b:5266:GLU:HG2   | 2.01                     | 0.91              |
| 22:b:6011:CLA:C1   | 22:b:6013:CLA:H93  | 1.99                     | 0.91              |
| 9:j:5010:LEU:HD13  | 9:j:5010:LEU:H     | 1.34                     | 0.91              |
| 1:A:310:LYS:HB2    | 16:V:28:GLU:HB3    | 1.51                     | 0.91              |
| 22:B:1016:CLA:HBC3 | 22:B:1016:CLA:HHD  | 1.49                     | 0.91              |
| 23:D:1039:PHO:HBA2 | 23:D:1039:PHO:HMA1 | 1.47                     | 0.91              |
| 16:V:88:ALA:HA     | 16:V:108:TYR:CE2   | 2.05                     | 0.91              |
| 1:a:5279:ARG:CD    | 4:d:5208:ALA:HB1   | 1.98                     | 0.91              |
| 22:b:6021:CLA:HMD2 | 22:b:6022:CLA:HBB2 | 1.52                     | 0.91              |
| 22:c:6031:CLA:OBD  | 22:c:6033:CLA:H161 | 1.71                     | 0.91              |
| 1:a:5076:ASN:ND2   | 11:l:5033:SER:HB3  | 1.85                     | 0.91              |
| 22:A:1003:CLA:H42  | 23:A:1038:PHO:NB   | 1.85                     | 0.91              |
| 2:B:174:LEU:CD2    | 2:B:266:GLU:HG2    | 2.01                     | 0.91              |
| 3:C:36:TRP:CZ3     | 3:C:37:ALA:HB2     | 2.06                     | 0.91              |
| 22:C:1031:CLA:OBD  | 22:C:1033:CLA:H161 | 1.71                     | 0.91              |
| 22:C:1035:CLA:HBB2 | 22:K:1034:CLA:HMA2 | 1.48                     | 0.91              |
| 3:c:5049:LEU:CD2   | 3:c:5052:ALA:N     | 2.28                     | 0.91              |
| 22:B:1015:CLA:C4   | 22:B:1015:CLA:H71  | 2.00                     | 0.91              |
| 22:D:1005:CLA:HBC1 | 22:D:1004:CLA:HBB2 | 1.48                     | 0.91              |
| 4:d:5139:ARG:HH12  | 4:d:5265:ARG:HH21  | 1.14                     | 0.91              |
| 23:d:6039:PHO:HMA2 | 22:d:6004:CLA:H143 | 1.50                     | 0.91              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1022:CLA:H202 | 22:B:1022:CLA:C2D  | 2.01                     | 0.91              |
| 20:Z:20:VAL:O      | 20:Z:24:PRO:HD2    | 1.69                     | 0.91              |
| 1:a:5314:ILE:HD12  | 4:d:5058:TRP:HZ3   | 1.36                     | 0.91              |
| 22:b:6016:CLA:H52  | 22:h:6017:CLA:H92  | 1.48                     | 0.91              |
| 29:C:1055:DGD:HAT1 | 29:C:1055:DGD:C6A  | 2.01                     | 0.91              |
| 22:b:6021:CLA:HED3 | 22:b:6021:CLA:O1A  | 1.70                     | 0.91              |
| 3:c:5049:LEU:O     | 3:c:5049:LEU:HD13  | 1.71                     | 0.91              |
| 3:c:5100:GLY:HA2   | 3:c:5196:VAL:HG12  | 1.50                     | 0.91              |
| 13:o:5052:ALA:HB1  | 13:o:5230:VAL:H    | 1.34                     | 0.91              |
| 22:b:6022:CLA:H143 | 22:b:6022:CLA:H101 | 1.51                     | 0.91              |
| 22:b:6023:CLA:H101 | 22:b:6023:CLA:H161 | 1.51                     | 0.91              |
| 29:b:6058:DGD:HB2  | 29:b:6058:DGD:HBG2 | 0.91                     | 0.91              |
| 3:c:5056:HIS:C     | 3:c:5058:GLY:H     | 1.72                     | 0.91              |
| 25:k:6051:BCR:H23C | 25:k:6051:BCR:C40  | 2.01                     | 0.91              |
| 22:B:1021:CLA:HMD2 | 22:B:1022:CLA:HBB2 | 1.52                     | 0.91              |
| 3:C:224:ILE:HD12   | 25:C:1054:BCR:H383 | 1.53                     | 0.91              |
| 3:C:296:VAL:HG23   | 3:C:297:TYR:CD1    | 2.06                     | 0.91              |
| 22:D:1008:CLA:CBA  | 22:D:1008:CLA:HMA3 | 2.01                     | 0.91              |
| 13:O:214:LYS:HE3   | 13:O:251:MET:HG3   | 1.53                     | 0.91              |
| 2:b:5273:TYR:HA    | 2:b:5276:ASP:OD1   | 1.71                     | 0.91              |
| 3:c:5224:ILE:HD12  | 25:c:6054:BCR:H383 | 1.53                     | 0.91              |
| 22:c:6032:CLA:HAB  | 22:k:6034:CLA:HMC1 | 1.53                     | 0.91              |
| 23:d:6039:PHO:HMA3 | 22:d:6004:CLA:C14  | 2.01                     | 0.91              |
| 22:A:1003:CLA:C4   | 23:A:1038:PHO:C1B  | 2.49                     | 0.90              |
| 28:B:1060:MGE:H7B1 | 28:B:1060:MGE:H3B2 | 1.53                     | 0.90              |
| 29:C:1057:DGD:CIB  | 29:C:1057:DGD:CEB  | 2.47                     | 0.90              |
| 25:Z:1053:BCR:H361 | 25:Z:1053:BCR:C37  | 2.01                     | 0.90              |
| 3:c:5117:VAL:HG11  | 22:c:6027:CLA:H42  | 1.50                     | 0.90              |
| 22:c:6036:CLA:HBB1 | 22:c:6036:CLA:HHC  | 1.53                     | 0.90              |
| 23:d:6039:PHO:HMA3 | 22:d:6004:CLA:H102 | 1.50                     | 0.90              |
| 22:a:6003:CLA:C4   | 23:a:6038:PHO:C1B  | 2.49                     | 0.90              |
| 24:a:6043:PQ9:H452 | 28:d:6059:MGE:C8A  | 2.01                     | 0.90              |
| 22:b:6021:CLA:H2   | 22:b:6021:CLA:HMA3 | 1.52                     | 0.90              |
| 3:c:5348:GLU:HG2   | 3:c:5349:ILE:HG13  | 1.52                     | 0.90              |
| 16:v:5088:ALA:HA   | 16:v:5108:TYR:CE2  | 2.05                     | 0.90              |
| 25:z:6053:BCR:H361 | 25:z:6053:BCR:C37  | 2.02                     | 0.90              |
| 2:B:149:LEU:HB2    | 22:B:1012:CLA:H202 | 1.53                     | 0.90              |
| 2:B:273:TYR:HA     | 2:B:276:ASP:OD1    | 1.71                     | 0.90              |
| 22:C:1036:CLA:HHC  | 22:C:1036:CLA:HBB1 | 1.53                     | 0.90              |
| 22:b:6009:CLA:CBD  | 22:b:6010:CLA:HBB1 | 1.94                     | 0.90              |
| 6:f:5041:GLN:NE2   | 9:j:5028:PHE:HA    | 1.87                     | 0.90              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5184:ILE:HG12  | 4:d:5186:GLN:NE2   | 1.87                     | 0.90              |
| 1:A:279:ARG:HH11   | 23:A:1038:PHO:HMC2 | 0.76                     | 0.90              |
| 26:A:1063:LHG:C29  | 22:C:1032:CLA:C7   | 2.50                     | 0.90              |
| 22:B:1009:CLA:CED  | 22:B:1009:CLA:H2A  | 2.00                     | 0.90              |
| 22:B:1022:CLA:H143 | 22:B:1022:CLA:H101 | 1.51                     | 0.90              |
| 16:V:62:ALA:O      | 16:V:63:CYS:HB2    | 1.70                     | 0.90              |
| 2:b:5105:GLY:HA2   | 25:b:6047:BCR:C40  | 2.02                     | 0.90              |
| 22:b:6022:CLA:C2D  | 22:b:6022:CLA:H202 | 2.01                     | 0.90              |
| 4:D:261:PHE:H      | 24:D:1042:PQ9:C9   | 1.85                     | 0.90              |
| 13:O:52:ALA:HB1    | 13:O:230:VAL:H     | 1.34                     | 0.90              |
| 1:a:5220:THR:HA    | 1:a:5223:LEU:HD23  | 1.54                     | 0.90              |
| 3:C:61:VAL:HG11    | 3:C:125:LEU:HD13   | 1.53                     | 0.90              |
| 3:C:100:GLY:HA2    | 3:C:196:VAL:HG12   | 1.50                     | 0.90              |
| 29:C:1057:DGD:HAF2 | 28:D:1059:MGE:CCB  | 1.99                     | 0.90              |
| 2:b:5174:LEU:N     | 2:b:5174:LEU:CD1   | 2.35                     | 0.90              |
| 16:v:5062:ALA:O    | 16:v:5063:CYS:HB2  | 1.70                     | 0.90              |
| 22:C:1033:CLA:H2   | 22:C:1033:CLA:O1A  | 1.72                     | 0.90              |
| 1:a:5180:PHE:CD1   | 4:d:5192:THR:HB    | 2.07                     | 0.90              |
| 22:b:6009:CLA:H8   | 22:b:6009:CLA:H143 | 0.90                     | 0.90              |
| 1:A:127:MET:O      | 1:A:130:GLN:HB3    | 1.72                     | 0.90              |
| 1:A:180:PHE:CD1    | 4:D:192:THR:HB     | 2.07                     | 0.90              |
| 1:A:184:ILE:HG12   | 4:D:186:GLN:NE2    | 1.87                     | 0.90              |
| 1:A:224:ILE:H      | 2:B:482:ILE:HG23   | 1.34                     | 0.90              |
| 22:B:1023:CLA:H13  | 22:B:1024:CLA:HMA1 | 1.50                     | 0.90              |
| 1:a:5316:THR:C     | 4:d:5063:LEU:HD21  | 1.97                     | 0.90              |
| 29:c:6057:DGD:CIB  | 29:c:6057:DGD:CEB  | 2.47                     | 0.90              |
| 2:B:65:PHE:HE2     | 22:B:1012:CLA:HMA2 | 1.23                     | 0.90              |
| 22:B:1022:CLA:H43  | 22:B:1022:CLA:CGA  | 2.01                     | 0.90              |
| 3:C:49:LEU:O       | 3:C:49:LEU:HD13    | 1.71                     | 0.90              |
| 11:L:14:ARG:HA     | 12:M:26:TYR:HE1    | 1.36                     | 0.90              |
| 2:b:5149:LEU:HB2   | 22:b:6012:CLA:H202 | 1.53                     | 0.90              |
| 3:C:199:ILE:HG21   | 3:C:234:VAL:HG11   | 1.54                     | 0.89              |
| 3:C:449:ARG:HD3    | 22:C:1029:CLA:HED1 | 1.54                     | 0.89              |
| 5:E:13:ILE:HG12    | 31:F:1040:HEM:HBC2 | 1.52                     | 0.89              |
| 11:L:24:ILE:HD13   | 12:M:18:PRO:HG2    | 1.52                     | 0.89              |
| 22:A:1006:CLA:HHH  | 22:A:1006:CLA:CBC  | 2.02                     | 0.89              |
| 2:B:265:ILE:HD12   | 2:B:265:ILE:H      | 1.36                     | 0.89              |
| 4:D:253:TRP:HA     | 4:D:256:ILE:CG2    | 2.02                     | 0.89              |
| 24:A:1043:PQ9:H452 | 28:D:1059:MGE:C8A  | 2.01                     | 0.89              |
| 22:C:1033:CLA:CMA  | 22:K:1034:CLA:C2C  | 2.51                     | 0.89              |
| 23:D:1039:PHO:HMA3 | 22:D:1004:CLA:C14  | 2.01                     | 0.89              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5338:GLN:HE21  | 2:b:5338:GLN:HA    | 1.36                     | 0.89              |
| 22:c:6031:CLA:H141 | 25:c:6054:BCR:H362 | 1.55                     | 0.89              |
| 4:d:5226:GLY:HA3   | 4:d:5234:ALA:HB2   | 1.54                     | 0.89              |
| 15:u:5031:ASN:HD22 | 15:u:5032:ILE:N    | 1.70                     | 0.89              |
| 28:B:1060:MGE:CFB  | 28:B:1060:MGE:CBB  | 2.32                     | 0.89              |
| 3:C:48:LYS:HD2     | 22:C:1035:CLA:HED1 | 1.53                     | 0.89              |
| 4:D:226:GLY:HA3    | 4:D:234:ALA:HB2    | 1.54                     | 0.89              |
| 22:D:1008:CLA:H143 | 22:D:1008:CLA:H18  | 1.52                     | 0.89              |
| 22:B:1009:CLA:H8   | 22:B:1009:CLA:H143 | 0.90                     | 0.89              |
| 28:B:1060:MGE:H7B1 | 28:B:1060:MGE:C3B  | 2.03                     | 0.89              |
| 22:D:1008:CLA:HBA1 | 22:D:1008:CLA:HMA3 | 1.54                     | 0.89              |
| 22:b:6014:CLA:HHD  | 22:b:6014:CLA:CBC  | 2.00                     | 0.89              |
| 11:l:5029:LEU:HB2  | 14:t:5009:ILE:HG21 | 1.54                     | 0.89              |
| 8:I:31:ASN:HB2     | 8:I:32:PRO:HD2     | 1.55                     | 0.89              |
| 22:b:6022:CLA:CGA  | 22:b:6022:CLA:H43  | 2.01                     | 0.89              |
| 4:d:5261:PHE:H     | 24:d:6042:PQ9:C9   | 1.85                     | 0.89              |
| 22:d:6008:CLA:H143 | 22:d:6008:CLA:H18  | 1.52                     | 0.89              |
| 3:c:5117:VAL:HG12  | 3:c:5118:HIS:N     | 1.87                     | 0.89              |
| 3:c:5449:ARG:HD3   | 22:c:6029:CLA:HED1 | 1.54                     | 0.89              |
| 22:c:6033:CLA:CMA  | 22:k:6034:CLA:C2C  | 2.51                     | 0.89              |
| 29:c:6057:DGD:HB2  | 29:c:6057:DGD:HBG3 | 1.51                     | 0.89              |
| 25:A:1044:BCR:H403 | 25:A:1044:BCR:H372 | 1.55                     | 0.89              |
| 26:A:1063:LHG:C29  | 22:C:1032:CLA:H72  | 2.01                     | 0.89              |
| 22:C:1025:CLA:C12  | 25:C:1054:BCR:C35  | 2.49                     | 0.89              |
| 6:F:41:GLN:NE2     | 9:J:28:PHE:HA      | 1.87                     | 0.89              |
| 25:T:6046:BCR:H392 | 25:T:6046:BCR:H23C | 1.54                     | 0.89              |
| 25:T:6046:BCR:C35  | 25:b:6047:BCR:H24C | 2.02                     | 0.89              |
| 22:b:6015:CLA:C4   | 22:b:6015:CLA:H71  | 2.00                     | 0.89              |
| 22:b:6016:CLA:H51  | 22:h:6017:CLA:H112 | 1.52                     | 0.89              |
| 2:B:127:ARG:HD3    | 2:B:128:THR:HG23   | 1.54                     | 0.89              |
| 2:B:174:LEU:N      | 2:B:174:LEU:CD1    | 2.35                     | 0.89              |
| 2:B:338:GLN:HA     | 2:B:338:GLN:HE21   | 1.36                     | 0.89              |
| 2:B:460:LEU:HA     | 29:B:1058:DGD:HAG1 | 1.53                     | 0.89              |
| 22:B:1023:CLA:H91  | 22:B:1024:CLA:C15  | 2.03                     | 0.89              |
| 25:B:1047:BCR:H24C | 25:t:1046:BCR:C35  | 2.02                     | 0.89              |
| 1:a:5265:PHE:CZ    | 26:a:6063:LHG:H151 | 2.07                     | 0.89              |
| 4:d:5253:TRP:HA    | 4:d:5256:ILE:CG2   | 2.02                     | 0.89              |
| 23:A:1038:PHO:C20  | 22:D:1005:CLA:HMB1 | 2.03                     | 0.89              |
| 3:c:5223:TRP:CD1   | 3:c:5224:ILE:HG12  | 2.08                     | 0.89              |
| 3:c:5296:VAL:HG23  | 3:c:5297:TYR:CD1   | 2.06                     | 0.89              |
| 22:d:6008:CLA:HBA1 | 22:d:6008:CLA:HMA3 | 1.54                     | 0.89              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:191:ASN:ND2    | 7:H:60:VAL:HG12    | 1.88                     | 0.88              |
| 22:B:1012:CLA:H12  | 22:B:1013:CLA:H43  | 1.55                     | 0.88              |
| 22:B:1013:CLA:HAB  | 22:B:1014:CLA:C5   | 2.03                     | 0.88              |
| 22:d:6008:CLA:CBA  | 22:d:6008:CLA:HMA3 | 2.01                     | 0.88              |
| 1:A:314:ILE:HD12   | 4:D:58:TRP:HZ3     | 1.36                     | 0.88              |
| 1:A:316:THR:C      | 4:D:63:LEU:HD21    | 1.97                     | 0.88              |
| 3:C:223:TRP:CD1    | 3:C:224:ILE:HG12   | 2.08                     | 0.88              |
| 24:D:1042:PQ9:O1   | 24:D:1042:PQ9:H143 | 1.72                     | 0.88              |
| 13:O:132:VAL:HG23  | 13:O:144:LEU:HD21  | 1.55                     | 0.88              |
| 22:a:6003:CLA:HAA2 | 22:a:6003:CLA:HED3 | 1.54                     | 0.88              |
| 2:b:5025:MET:HG3   | 25:b:6045:BCR:H401 | 1.55                     | 0.88              |
| 3:c:5048:LYS:HD2   | 22:c:6035:CLA:HED1 | 1.53                     | 0.88              |
| 3:c:5061:VAL:HG11  | 3:c:5125:LEU:HD13  | 1.53                     | 0.88              |
| 10:k:5033:PHE:CD1  | 10:k:5033:PHE:C    | 2.49                     | 0.88              |
| 11:l:5024:ILE:HD13 | 12:m:5018:PRO:HG2  | 1.52                     | 0.88              |
| 2:B:311:PHE:HE2    | 2:B:317:ASN:HD21   | 1.15                     | 0.88              |
| 10:K:33:PHE:C      | 10:K:33:PHE:CD2    | 2.50                     | 0.88              |
| 12:M:9:ILE:CD1     | 12:m:5009:ILE:CD1  | 2.51                     | 0.88              |
| 22:b:6021:CLA:CED  | 22:b:6021:CLA:H2   | 2.03                     | 0.88              |
| 28:b:6060:MGE:H3B2 | 28:b:6060:MGE:H7B1 | 1.53                     | 0.88              |
| 24:d:6042:PQ9:H143 | 24:d:6042:PQ9:O1   | 1.72                     | 0.88              |
| 22:B:1015:CLA:CAC  | 25:t:1046:BCR:H281 | 2.03                     | 0.88              |
| 29:B:1058:DGD:HB2  | 29:B:1058:DGD:HBG2 | 0.91                     | 0.88              |
| 3:C:348:GLU:HG2    | 3:C:349:ILE:HG13   | 1.52                     | 0.88              |
| 22:C:1035:CLA:C8   | 25:C:1052:BCR:C40  | 2.52                     | 0.88              |
| 4:D:191:TRP:CE2    | 4:D:197:HIS:HB2    | 2.08                     | 0.88              |
| 1:a:5279:ARG:HH21  | 23:a:6038:PHO:CMC  | 1.85                     | 0.88              |
| 2:b:5460:LEU:HA    | 29:b:6058:DGD:HAG1 | 1.53                     | 0.88              |
| 3:c:5063:TRP:HE1   | 22:c:6028:CLA:C2C  | 1.86                     | 0.88              |
| 8:i:5031:ASN:HB2   | 8:i:5032:PRO:HD2   | 1.55                     | 0.88              |
| 22:B:1021:CLA:CED  | 22:B:1021:CLA:H2   | 2.04                     | 0.88              |
| 2:b:5127:ARG:HD3   | 2:b:5128:THR:HG23  | 1.54                     | 0.88              |
| 22:c:6029:CLA:HBA2 | 22:c:6029:CLA:CMA  | 2.03                     | 0.88              |
| 4:d:5124:GLY:HA2   | 4:d:5127:LEU:HD12  | 1.54                     | 0.88              |
| 2:B:99:ALA:HB1     | 22:B:1014:CLA:C4   | 2.04                     | 0.88              |
| 25:T:6046:BCR:H281 | 22:b:6015:CLA:CAC  | 2.03                     | 0.88              |
| 26:a:6063:LHG:C29  | 22:c:6032:CLA:C7   | 2.51                     | 0.88              |
| 2:b:5191:ASN:ND2   | 7:h:5060:VAL:HG12  | 1.88                     | 0.88              |
| 22:b:6012:CLA:H12  | 22:b:6013:CLA:H43  | 1.55                     | 0.88              |
| 11:l:5014:ARG:HA   | 12:m:5026:TYR:HE1  | 1.36                     | 0.88              |
| 2:B:25:MET:HG3     | 25:B:1045:BCR:H401 | 1.55                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:56:HIS:HA      | 3:C:59:LEU:HD12    | 1.56                     | 0.88              |
| 3:C:117:VAL:HG12   | 3:C:118:HIS:N      | 1.87                     | 0.88              |
| 22:C:1029:CLA:HBA2 | 22:C:1029:CLA:CMA  | 2.03                     | 0.88              |
| 22:C:1031:CLA:H141 | 25:C:1054:BCR:H362 | 1.54                     | 0.88              |
| 28:b:6060:MGE:H7B1 | 28:b:6060:MGE:C3B  | 2.03                     | 0.88              |
| 3:c:5039:ASN:HB2   | 22:c:6032:CLA:HBA1 | 1.56                     | 0.88              |
| 22:C:1033:CLA:HMA1 | 22:K:1034:CLA:C2C  | 2.04                     | 0.88              |
| 25:D:1050:BCR:H383 | 25:D:1050:BCR:C23  | 1.97                     | 0.88              |
| 3:c:5140:LEU:HD21  | 3:c:5146:PHE:HE1   | 1.38                     | 0.88              |
| 22:c:6025:CLA:C12  | 25:c:6054:BCR:C35  | 2.49                     | 0.88              |
| 25:t:1046:BCR:H392 | 25:t:1046:BCR:H23C | 1.54                     | 0.88              |
| 2:B:7:ARG:HG2      | 2:B:7:ARG:NH1      | 1.83                     | 0.88              |
| 2:B:105:GLY:HA3    | 25:B:1047:BCR:C40  | 2.02                     | 0.88              |
| 22:B:1012:CLA:CBB  | 22:B:1015:CLA:HBB2 | 2.04                     | 0.88              |
| 4:D:183:LEU:HD23   | 4:D:183:LEU:H      | 1.38                     | 0.88              |
| 10:K:31:LEU:HB3    | 25:K:1051:BCR:C14  | 2.03                     | 0.88              |
| 2:b:5265:ILE:H     | 2:b:5265:ILE:HD12  | 1.36                     | 0.88              |
| 22:b:6013:CLA:HAB  | 22:b:6014:CLA:C5   | 2.03                     | 0.88              |
| 3:c:5050:LEU:HD21  | 3:c:5054:VAL:HG23  | 1.54                     | 0.88              |
| 22:c:6025:CLA:H91  | 25:c:6054:BCR:H373 | 1.56                     | 0.88              |
| 1:A:220:THR:HA     | 1:A:223:LEU:HD23   | 1.53                     | 0.87              |
| 1:A:265:PHE:CZ     | 26:A:1063:LHG:H151 | 2.07                     | 0.87              |
| 25:B:1048:BCR:H403 | 25:B:1048:BCR:H372 | 1.56                     | 0.87              |
| 4:D:124:GLY:HA2    | 4:D:127:LEU:HD12   | 1.54                     | 0.87              |
| 11:L:29:LEU:HB2    | 14:T:9:ILE:HG21    | 1.54                     | 0.87              |
| 15:U:31:ASN:HD22   | 15:U:32:ILE:N      | 1.70                     | 0.87              |
| 18:Y:43:ARG:CG     | 18:Y:44:GLY:H      | 1.87                     | 0.87              |
| 1:a:5127:MET:O     | 1:a:5130:GLN:HB3   | 1.72                     | 0.87              |
| 2:b:5099:ALA:HB1   | 22:b:6014:CLA:C4   | 2.04                     | 0.87              |
| 22:c:6025:CLA:H141 | 22:c:6031:CLA:CMB  | 2.05                     | 0.87              |
| 13:o:5055:ALA:HB1  | 13:o:5161:SER:HB3  | 1.55                     | 0.87              |
| 22:B:1020:CLA:H102 | 22:B:1020:CLA:C16  | 2.03                     | 0.87              |
| 29:c:6056:DGD:O1A  | 29:c:6056:DGD:HA41 | 1.73                     | 0.87              |
| 4:d:5191:TRP:CE2   | 4:d:5197:HIS:HB2   | 2.08                     | 0.87              |
| 10:k:5031:LEU:HB3  | 25:k:6051:BCR:C14  | 2.03                     | 0.87              |
| 13:o:5214:LYS:HE3  | 13:o:5251:MET:HG3  | 1.53                     | 0.87              |
| 3:C:39:ASN:HB2     | 22:C:1032:CLA:HBA1 | 1.56                     | 0.87              |
| 18:Y:42:ARG:HB3    | 18:Y:43:ARG:HH11   | 1.40                     | 0.87              |
| 22:a:6006:CLA:HHD  | 22:a:6006:CLA:CBC  | 2.02                     | 0.87              |
| 22:c:6029:CLA:C4B  | 22:c:6029:CLA:C5   | 2.52                     | 0.87              |
| 22:c:6035:CLA:C8   | 25:k:6052:BCR:C40  | 2.52                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5274:VAL:HB    | 4:d:5275:PRO:HD3   | 1.55                     | 0.87              |
| 6:f:5019:ARG:HH22  | 31:f:6040:HEM:HAC  | 1.39                     | 0.87              |
| 25:t:1046:BCR:H331 | 25:t:1046:BCR:C8   | 1.92                     | 0.87              |
| 22:B:1011:CLA:C19  | 22:H:1017:CLA:C10  | 2.51                     | 0.87              |
| 22:B:1018:CLA:H152 | 22:B:1020:CLA:O1A  | 1.75                     | 0.87              |
| 3:C:50:LEU:HD21    | 3:C:54:VAL:HG23    | 1.54                     | 0.87              |
| 3:C:63:TRP:HE1     | 22:C:1028:CLA:C2C  | 1.86                     | 0.87              |
| 3:C:79:LYS:HB3     | 3:C:84:GLN:NE2     | 1.89                     | 0.87              |
| 22:C:1032:CLA:HAB  | 22:K:1034:CLA:HMC1 | 1.53                     | 0.87              |
| 22:b:6011:CLA:C19  | 22:h:6017:CLA:C10  | 2.51                     | 0.87              |
| 22:b:6023:CLA:H91  | 22:b:6024:CLA:C15  | 2.03                     | 0.87              |
| 22:c:6033:CLA:O1A  | 22:c:6033:CLA:H2   | 1.72                     | 0.87              |
| 22:A:1003:CLA:HAA2 | 22:A:1003:CLA:HED3 | 1.54                     | 0.87              |
| 4:D:258:GLY:O      | 4:D:259:ILE:HD13   | 1.73                     | 0.87              |
| 2:b:5332:LYS:HB3   | 2:b:5444:ARG:HH12  | 1.38                     | 0.87              |
| 25:b:6047:BCR:H392 | 25:b:6047:BCR:H373 | 1.56                     | 0.87              |
| 4:d:5183:LEU:HD23  | 4:d:5183:LEU:H     | 1.38                     | 0.87              |
| 4:d:5258:GLY:O     | 4:d:5259:ILE:HD13  | 1.73                     | 0.87              |
| 22:B:1018:CLA:C10  | 22:B:1023:CLA:CAA  | 2.52                     | 0.87              |
| 3:C:417:VAL:CG1    | 16:V:68:VAL:HB     | 2.05                     | 0.87              |
| 22:C:1029:CLA:C4B  | 22:C:1029:CLA:C5   | 2.52                     | 0.87              |
| 5:E:20:TRP:HZ2     | 9:J:13:VAL:HG23    | 1.40                     | 0.87              |
| 25:H:1049:BCR:H311 | 25:H:1049:BCR:HC8  | 1.57                     | 0.87              |
| 1:a:5325:ASN:HD22  | 1:a:5328:MET:HE3   | 1.39                     | 0.87              |
| 2:b:5456:ALA:CB    | 29:b:6058:DGD:HBV1 | 2.05                     | 0.87              |
| 22:b:6021:CLA:H2A  | 22:b:6021:CLA:O1A  | 1.61                     | 0.87              |
| 29:c:6055:DGD:C6A  | 29:c:6055:DGD:HAT1 | 2.01                     | 0.87              |
| 15:u:5068:THR:CG2  | 15:u:5071:GLN:H    | 1.86                     | 0.87              |
| 2:B:133:LEU:HD23   | 2:B:138:MET:HE1    | 1.57                     | 0.87              |
| 2:B:191:ASN:HD21   | 7:H:60:VAL:HA      | 1.39                     | 0.87              |
| 2:B:332:LYS:HB3    | 2:B:444:ARG:HH12   | 1.38                     | 0.87              |
| 5:e:5073:LYS:O     | 5:e:5076:VAL:HG23  | 1.74                     | 0.87              |
| 18:y:5032:GLY:O    | 18:y:5035:ILE:HG23 | 1.75                     | 0.87              |
| 25:B:1048:BCR:H392 | 25:B:1048:BCR:H373 | 1.56                     | 0.87              |
| 4:D:92:LEU:HA      | 4:D:104:TRP:CD1    | 2.09                     | 0.87              |
| 5:E:73:LYS:O       | 5:E:76:VAL:HG23    | 1.74                     | 0.87              |
| 15:U:45:LEU:O      | 15:U:49:ILE:HG13   | 1.74                     | 0.87              |
| 15:U:68:THR:CG2    | 15:U:71:GLN:H      | 1.86                     | 0.87              |
| 25:a:6044:BCR:H392 | 25:a:6044:BCR:H373 | 1.55                     | 0.87              |
| 25:a:6044:BCR:H403 | 25:a:6044:BCR:H372 | 1.55                     | 0.87              |
| 11:l:5014:ARG:HA   | 12:m:5026:TYR:CE1  | 2.10                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:H:44:ILE:HD11    | 17:X:19:PHE:CE2    | 2.10                     | 0.87              |
| 25:K:1051:BCR:H23C | 25:K:1051:BCR:C40  | 2.01                     | 0.87              |
| 22:b:6011:CLA:C2   | 22:b:6013:CLA:C9   | 2.53                     | 0.87              |
| 3:c:5223:TRP:NE1   | 3:c:5224:ILE:HG12  | 1.90                     | 0.87              |
| 10:k:5033:PHE:C    | 10:k:5033:PHE:HD1  | 1.80                     | 0.87              |
| 15:u:5045:LEU:O    | 15:u:5049:ILE:HG13 | 1.74                     | 0.87              |
| 22:B:1011:CLA:C2   | 22:B:1013:CLA:C9   | 2.53                     | 0.86              |
| 22:B:1014:CLA:H111 | 25:B:1048:BCR:HC7  | 1.57                     | 0.86              |
| 22:B:1023:CLA:H143 | 22:B:1024:CLA:H61  | 1.57                     | 0.86              |
| 13:o:5132:VAL:HG23 | 13:o:5144:LEU:HD21 | 1.55                     | 0.86              |
| 4:D:274:VAL:HB     | 4:D:275:PRO:HD3    | 1.55                     | 0.86              |
| 13:O:85:LYS:HB3    | 2:b:5307:GLU:OE2   | 1.75                     | 0.86              |
| 18:Y:32:GLY:O      | 18:Y:35:ILE:HG23   | 1.74                     | 0.86              |
| 2:b:5223:GLN:HE21  | 7:h:5021:VAL:HG11  | 1.39                     | 0.86              |
| 22:b:6018:CLA:C10  | 22:b:6023:CLA:CAA  | 2.52                     | 0.86              |
| 3:c:5264:PHE:N     | 3:c:5264:PHE:CD2   | 2.30                     | 0.86              |
| 4:d:5092:LEU:HA    | 4:d:5104:TRP:CD1   | 2.09                     | 0.86              |
| 4:d:5095:PRO:HG3   | 17:x:5015:SER:HB2  | 1.57                     | 0.86              |
| 1:A:44:ALA:HB2     | 1:A:118:HIS:HB3    | 1.57                     | 0.86              |
| 22:A:1003:CLA:C4   | 23:A:1038:PHO:C2B  | 2.52                     | 0.86              |
| 2:B:65:PHE:CZ      | 22:B:1012:CLA:HMA3 | 2.10                     | 0.86              |
| 22:C:1028:CLA:H102 | 29:C:1056:DGD:HAS2 | 1.57                     | 0.86              |
| 29:C:1056:DGD:O1A  | 29:C:1056:DGD:HA41 | 1.73                     | 0.86              |
| 6:F:40:MET:O       | 6:F:43:ILE:HG13    | 1.75                     | 0.86              |
| 22:K:1034:CLA:C4   | 22:K:1034:CLA:C7   | 2.49                     | 0.86              |
| 1:a:5279:ARG:HD3   | 4:d:5208:ALA:HB1   | 1.55                     | 0.86              |
| 3:c:5049:LEU:CD2   | 3:c:5052:ALA:CB    | 2.53                     | 0.86              |
| 3:c:5079:LYS:HB3   | 3:c:5084:GLN:NE2   | 1.89                     | 0.86              |
| 22:c:6033:CLA:HMA1 | 22:k:6034:CLA:C2C  | 2.04                     | 0.86              |
| 2:B:223:GLN:HE21   | 7:H:21:VAL:HG11    | 1.39                     | 0.86              |
| 12:M:9:ILE:HG12    | 12:m:5008:PHE:HB3  | 1.57                     | 0.86              |
| 22:b:6012:CLA:C1D  | 22:b:6020:CLA:H201 | 2.05                     | 0.86              |
| 22:b:6013:CLA:C12  | 22:b:6018:CLA:H42  | 2.05                     | 0.86              |
| 3:c:5199:ILE:HG21  | 3:c:5234:VAL:HG11  | 1.54                     | 0.86              |
| 4:d:5213:ILE:HG12  | 24:d:6042:PQ9:H111 | 1.58                     | 0.86              |
| 6:f:5015:ILE:HG13  | 6:f:5016:PHE:HD1   | 1.41                     | 0.86              |
| 22:A:1003:CLA:H42  | 23:A:1038:PHO:C2B  | 2.06                     | 0.86              |
| 2:B:456:ALA:CB     | 29:B:1058:DGD:HBV1 | 2.05                     | 0.86              |
| 3:C:172:ALA:N      | 22:C:1025:CLA:HBC2 | 1.90                     | 0.86              |
| 10:K:11:LEU:HD11   | 10:K:22:VAL:HG21   | 1.58                     | 0.86              |
| 23:a:6038:PHO:C20  | 22:d:6005:CLA:HMB1 | 2.03                     | 0.86              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6012:CLA:CBB  | 22:b:6015:CLA:HBB2 | 2.04                     | 0.86              |
| 1:A:297:LEU:HD22   | 3:C:404:LEU:HD23   | 1.56                     | 0.86              |
| 2:B:105:GLY:HA2    | 25:B:1047:BCR:C40  | 2.02                     | 0.86              |
| 3:C:49:LEU:CD2     | 3:C:52:ALA:CB      | 2.53                     | 0.86              |
| 25:T:6048:BCR:H403 | 25:T:6048:BCR:H372 | 1.57                     | 0.86              |
| 1:a:5297:LEU:HD22  | 3:c:5404:LEU:HD23  | 1.56                     | 0.86              |
| 22:a:6003:CLA:H42  | 23:a:6038:PHO:C2B  | 2.06                     | 0.86              |
| 25:A:1044:BCR:H392 | 25:A:1044:BCR:H373 | 1.55                     | 0.86              |
| 7:H:54:ILE:O       | 7:H:55:LEU:HD13    | 1.75                     | 0.86              |
| 25:H:1049:BCR:C39  | 25:H:1049:BCR:C23  | 2.30                     | 0.86              |
| 2:b:5007:ARG:HG2   | 2:b:5007:ARG:NH1   | 1.83                     | 0.86              |
| 3:c:5042:LEU:CD2   | 3:c:5048:LYS:HG2   | 2.06                     | 0.86              |
| 3:c:5049:LEU:HD12  | 3:c:5049:LEU:N     | 1.91                     | 0.86              |
| 6:f:5040:MET:O     | 6:f:5043:ILE:HG13  | 1.75                     | 0.86              |
| 22:B:1013:CLA:C12  | 22:B:1018:CLA:H42  | 2.05                     | 0.86              |
| 3:C:49:LEU:HD12    | 3:C:49:LEU:N       | 1.91                     | 0.86              |
| 3:C:140:LEU:HD21   | 3:C:146:PHE:HE1    | 1.38                     | 0.86              |
| 3:C:223:TRP:NE1    | 3:C:224:ILE:HG12   | 1.90                     | 0.86              |
| 22:C:1035:CLA:C9   | 25:C:1052:BCR:H402 | 2.06                     | 0.86              |
| 22:K:1034:CLA:H71  | 22:K:1034:CLA:H43  | 1.57                     | 0.86              |
| 22:a:6003:CLA:C4   | 23:a:6038:PHO:C2B  | 2.52                     | 0.86              |
| 28:b:6060:MGE:CFB  | 28:b:6060:MGE:CBB  | 2.32                     | 0.86              |
| 3:c:5056:HIS:HA    | 3:c:5059:LEU:HD12  | 1.56                     | 0.86              |
| 3:c:5172:ALA:N     | 22:c:6025:CLA:HBC2 | 1.90                     | 0.86              |
| 3:c:5429:SER:HB3   | 29:c:6056:DGD:HA91 | 1.58                     | 0.86              |
| 22:c:6033:CLA:HMA2 | 22:k:6034:CLA:CAC  | 2.05                     | 0.86              |
| 13:o:5176:SER:HB3  | 13:o:5216:PHE:HE2  | 1.40                     | 0.86              |
| 15:u:5061:VAL:HG12 | 15:u:5075:LEU:HD23 | 1.58                     | 0.86              |
| 1:A:14:TRP:HH2     | 8:I:21:PHE:HB3     | 1.41                     | 0.86              |
| 1:A:103:ASP:HA     | 1:A:106:LEU:HD12   | 1.58                     | 0.86              |
| 4:D:95:PRO:HG3     | 17:X:15:SER:HB2    | 1.57                     | 0.86              |
| 4:D:160:TYR:CE1    | 27:D:1068:IOD:I    | 2.98                     | 0.86              |
| 28:D:1059:MGE:H251 | 28:D:1059:MGE:H212 | 1.56                     | 0.86              |
| 25:T:6048:BCR:H392 | 25:T:6048:BCR:H373 | 1.56                     | 0.86              |
| 2:b:5065:PHE:CZ    | 22:b:6012:CLA:CMA  | 2.58                     | 0.86              |
| 3:c:5263:ALA:CB    | 3:c:5264:PHE:CD2   | 2.59                     | 0.86              |
| 10:k:5026:PRO:O    | 10:k:5029:PRO:HD2  | 1.75                     | 0.86              |
| 3:C:49:LEU:HD11    | 22:C:1035:CLA:HMA2 | 1.57                     | 0.86              |
| 3:C:50:LEU:HD23    | 3:C:51:GLY:N       | 1.91                     | 0.86              |
| 3:C:263:ALA:CB     | 3:C:264:PHE:CD2    | 2.59                     | 0.86              |
| 3:C:429:SER:HB3    | 29:C:1056:DGD:HA91 | 1.58                     | 0.86              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:C:1056:DGD:C3E  | 29:C:1056:DGD:C6D  | 2.46                     | 0.86              |
| 13:O:55:ALA:HB1    | 13:O:161:SER:HB3   | 1.55                     | 0.86              |
| 1:a:5014:TRP:HH2   | 8:i:5021:PHE:HB3   | 1.41                     | 0.86              |
| 2:b:5105:GLY:HA3   | 25:b:6047:BCR:C40  | 2.02                     | 0.86              |
| 22:c:6037:CLA:HHD  | 22:c:6037:CLA:CBC  | 2.06                     | 0.86              |
| 7:h:5054:ILE:O     | 7:h:5055:LEU:HD13  | 1.75                     | 0.86              |
| 1:A:279:ARG:HD3    | 4:D:208:ALA:CB     | 2.06                     | 0.85              |
| 22:B:1016:CLA:C16  | 22:D:1008:CLA:CMA  | 2.30                     | 0.85              |
| 3:C:50:LEU:HD23    | 3:C:50:LEU:O       | 1.76                     | 0.85              |
| 4:D:213:ILE:HG12   | 24:D:1042:PQ9:H111 | 1.58                     | 0.85              |
| 10:K:26:PRO:O      | 10:K:29:PRO:HD2    | 1.75                     | 0.85              |
| 3:c:5417:VAL:CG1   | 16:v:5068:VAL:HB   | 2.05                     | 0.85              |
| 7:h:5044:ILE:HD11  | 17:x:5019:PHE:CE2  | 2.10                     | 0.85              |
| 22:B:1019:CLA:HBA1 | 22:B:1019:CLA:CHA  | 2.07                     | 0.85              |
| 3:C:42:LEU:CD1     | 3:C:49:LEU:CD1     | 2.54                     | 0.85              |
| 6:F:28:VAL:HB      | 6:F:29:PRO:HD3     | 1.58                     | 0.85              |
| 1:a:5044:ALA:HB2   | 1:a:5118:HIS:HB3   | 1.57                     | 0.85              |
| 22:b:6018:CLA:H152 | 22:b:6020:CLA:O1A  | 1.75                     | 0.85              |
| 5:e:5020:TRP:HZ2   | 9:j:5013:VAL:HG23  | 1.40                     | 0.85              |
| 1:A:258:LEU:HD12   | 4:D:128:ARG:NH2    | 1.91                     | 0.85              |
| 22:A:1006:CLA:C17  | 25:D:1050:BCR:H282 | 2.07                     | 0.85              |
| 22:B:1012:CLA:C1D  | 22:B:1020:CLA:H201 | 2.05                     | 0.85              |
| 25:B:1047:BCR:H392 | 25:B:1047:BCR:H373 | 1.56                     | 0.85              |
| 13:O:46:PRO:HB2    | 13:O:266:TYR:CD2   | 2.12                     | 0.85              |
| 1:a:5259:ILE:HD13  | 24:a:6043:PQ9:H242 | 1.58                     | 0.85              |
| 31:f:6040:HEM:HBB2 | 31:f:6040:HEM:HMB2 | 1.58                     | 0.85              |
| 18:y:5042:ARG:HB3  | 18:y:5043:ARG:HH11 | 1.40                     | 0.85              |
| 11:L:14:ARG:HA     | 12:M:26:TYR:CE1    | 2.10                     | 0.85              |
| 22:a:6006:CLA:C17  | 25:d:6050:BCR:H282 | 2.07                     | 0.85              |
| 2:b:5065:PHE:CZ    | 22:b:6012:CLA:HMA3 | 2.11                     | 0.85              |
| 22:b:6020:CLA:H102 | 22:b:6020:CLA:C16  | 2.03                     | 0.85              |
| 22:c:6035:CLA:C9   | 25:k:6052:BCR:H402 | 2.06                     | 0.85              |
| 24:d:6042:PQ9:H392 | 28:l:6061:MGE:H241 | 1.58                     | 0.85              |
| 22:B:1022:CLA:H93  | 22:B:1022:CLA:C13  | 2.05                     | 0.85              |
| 23:D:1039:PHO:HMA2 | 22:D:1004:CLA:C14  | 2.06                     | 0.85              |
| 13:O:179:THR:HG22  | 13:O:180:ALA:N     | 1.92                     | 0.85              |
| 2:b:5191:ASN:HD21  | 7:h:5060:VAL:HA    | 1.39                     | 0.85              |
| 1:A:259:ILE:HD13   | 24:A:1043:PQ9:H242 | 1.58                     | 0.85              |
| 1:A:325:ASN:HD22   | 1:A:328:MET:HE3    | 1.39                     | 0.85              |
| 25:b:6047:BCR:H403 | 25:b:6047:BCR:H372 | 1.56                     | 0.85              |
| 3:c:5050:LEU:HD23  | 3:c:5050:LEU:O     | 1.76                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6028:CLA:H102 | 29:c:6056:DGD:HAS2 | 1.57                     | 0.85              |
| 22:c:6033:CLA:C7   | 22:c:6033:CLA:C2   | 2.54                     | 0.85              |
| 13:o:5046:PRO:HB2  | 13:o:5266:TYR:CD2  | 2.12                     | 0.85              |
| 2:B:52:LEU:HD22    | 2:B:311:PHE:HD1    | 1.41                     | 0.85              |
| 22:C:1029:CLA:HMD1 | 22:C:1031:CLA:HAB  | 1.59                     | 0.85              |
| 13:O:132:VAL:HG23  | 13:O:144:LEU:CD2   | 2.07                     | 0.85              |
| 2:b:5133:LEU:HD23  | 2:b:5138:MET:HE1   | 1.57                     | 0.85              |
| 13:o:5132:VAL:HG23 | 13:o:5144:LEU:CD2  | 2.07                     | 0.85              |
| 1:A:52:PHE:CD2     | 1:A:71:LEU:HD11    | 2.11                     | 0.85              |
| 29:C:1055:DGD:HBFI | 29:C:1055:DGD:HGB2 | 1.58                     | 0.85              |
| 6:F:15:ILE:HG13    | 6:F:16:PHE:HD1     | 1.41                     | 0.85              |
| 25:T:6048:BCR:HC7  | 22:b:6014:CLA:H111 | 1.57                     | 0.85              |
| 22:b:6021:CLA:C10  | 22:b:6021:CLA:C14  | 2.34                     | 0.85              |
| 22:b:6022:CLA:H93  | 22:b:6022:CLA:C13  | 2.05                     | 0.85              |
| 22:k:6034:CLA:C4   | 22:k:6034:CLA:C7   | 2.49                     | 0.85              |
| 2:B:65:PHE:CZ      | 22:B:1012:CLA:CMA  | 2.58                     | 0.85              |
| 3:C:50:LEU:CD2     | 3:C:51:GLY:N       | 2.40                     | 0.85              |
| 1:a:5058:VAL:HG12  | 1:a:5060:ILE:H     | 1.42                     | 0.85              |
| 1:a:5149:ALA:HB3   | 1:a:5150:PRO:HD3   | 1.58                     | 0.85              |
| 3:c:5406:SER:HB3   | 29:c:6056:DGD:HE1  | 1.59                     | 0.85              |
| 2:B:3:LEU:HB3      | 11:L:9:PRO:O       | 1.77                     | 0.85              |
| 22:B:1012:CLA:CBB  | 22:B:1015:CLA:CBB  | 2.55                     | 0.85              |
| 22:C:1033:CLA:HMA2 | 22:K:1034:CLA:CAC  | 2.05                     | 0.85              |
| 1:a:5116:ILE:HD11  | 1:a:5158:PHE:HB3   | 1.59                     | 0.85              |
| 2:b:5463:PHE:HE1   | 22:b:6016:CLA:HBB1 | 1.42                     | 0.85              |
| 22:b:6011:CLA:HMD1 | 22:b:6013:CLA:H42  | 1.59                     | 0.85              |
| 7:H:43:LEU:HD21    | 17:X:19:PHE:CE1    | 2.12                     | 0.84              |
| 12:M:8:PHE:HB3     | 12:m:5009:ILE:HG12 | 1.59                     | 0.84              |
| 13:O:176:SER:HB3   | 13:O:216:PHE:HE2   | 1.41                     | 0.84              |
| 18:Y:42:ARG:CB     | 18:Y:43:ARG:HH11   | 1.90                     | 0.84              |
| 2:b:5055:MET:HE1   | 2:b:5080:ILE:HD13  | 1.58                     | 0.84              |
| 22:C:1030:CLA:HED2 | 22:C:1030:CLA:CAD  | 2.07                     | 0.84              |
| 10:K:33:PHE:O      | 10:K:33:PHE:CD2    | 2.30                     | 0.84              |
| 1:a:5077:ILE:HD11  | 14:t:5006:TYR:HB3  | 1.58                     | 0.84              |
| 1:a:5301:ASN:HD22  | 3:c:5407:VAL:HG11  | 1.41                     | 0.84              |
| 2:b:5149:LEU:HG    | 22:b:6011:CLA:CBC  | 2.05                     | 0.84              |
| 4:d:5184:PHE:HE2   | 4:d:5188:PHE:HD1   | 1.23                     | 0.84              |
| 6:f:5028:VAL:HB    | 6:f:5029:PRO:HD3   | 1.58                     | 0.84              |
| 20:z:5023:VAL:HG13 | 20:z:5027:TYR:CE2  | 2.12                     | 0.84              |
| 2:B:149:LEU:HG     | 22:B:1011:CLA:CBC  | 2.05                     | 0.84              |
| 3:C:406:SER:HB3    | 29:C:1056:DGD:HE1  | 1.59                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:D:1004:CLA:H201 | 28:D:1059:MGE:H8A1 | 1.58                     | 0.84              |
| 6:F:19:ARG:HH22    | 31:F:1040:HEM:HAC  | 1.39                     | 0.84              |
| 2:b:5463:PHE:CE1   | 22:b:6016:CLA:HBB1 | 2.12                     | 0.84              |
| 3:c:5050:LEU:CD2   | 3:c:5051:GLY:N     | 2.40                     | 0.84              |
| 25:d:6050:BCR:H383 | 25:d:6050:BCR:C23  | 1.97                     | 0.84              |
| 7:h:5043:LEU:HD21  | 17:x:5019:PHE:CE1  | 2.12                     | 0.84              |
| 25:h:6049:BCR:HC8  | 25:h:6049:BCR:H311 | 1.57                     | 0.84              |
| 18:y:5042:ARG:CB   | 18:y:5043:ARG:HH11 | 1.90                     | 0.84              |
| 22:C:1025:CLA:H91  | 25:C:1054:BCR:H373 | 1.56                     | 0.84              |
| 12:M:9:ILE:CD1     | 12:m:5009:ILE:HD11 | 2.07                     | 0.84              |
| 1:a:5052:PHE:CD2   | 1:a:5071:LEU:HD11  | 2.10                     | 0.84              |
| 23:a:6038:PHO:H2A  | 23:a:6038:PHO:O1D  | 1.77                     | 0.84              |
| 3:c:5229:ASN:HD22  | 3:c:5229:ASN:N     | 1.73                     | 0.84              |
| 4:d:5088:SER:HA    | 7:h:5050:ASN:ND2   | 1.93                     | 0.84              |
| 23:d:6039:PHO:CHD  | 23:d:6039:PHO:HBC2 | 2.06                     | 0.84              |
| 1:A:291:SER:HB3    | 3:C:431:PHE:CE1    | 2.13                     | 0.84              |
| 22:C:1037:CLA:HHD  | 22:C:1037:CLA:CBC  | 2.06                     | 0.84              |
| 25:b:6047:BCR:H371 | 25:b:6047:BCR:H392 | 1.32                     | 0.84              |
| 29:c:6056:DGD:C6D  | 29:c:6056:DGD:C5E  | 2.50                     | 0.84              |
| 1:a:5258:LEU:HD12  | 4:d:5128:ARG:NH2   | 1.91                     | 0.84              |
| 3:c:5049:LEU:H     | 3:c:5049:LEU:CD1   | 1.90                     | 0.84              |
| 18:y:5043:ARG:CG   | 18:y:5044:GLY:H    | 1.87                     | 0.84              |
| 1:A:338:ASN:O      | 1:A:339:PHE:CG     | 2.30                     | 0.84              |
| 23:a:6038:PHO:H202 | 22:d:6005:CLA:CMB  | 2.07                     | 0.84              |
| 2:b:5220:ARG:HD2   | 7:h:5020:LYS:O     | 1.76                     | 0.84              |
| 2:b:5460:LEU:O     | 2:b:5460:LEU:HD23  | 1.77                     | 0.84              |
| 22:b:6019:CLA:C19  | 22:b:6021:CLA:H72  | 2.07                     | 0.84              |
| 22:b:6022:CLA:H142 | 22:b:6022:CLA:C6   | 1.98                     | 0.84              |
| 22:b:6023:CLA:H143 | 22:b:6024:CLA:H61  | 1.57                     | 0.84              |
| 23:d:6039:PHO:HMA2 | 22:d:6004:CLA:C14  | 2.06                     | 0.84              |
| 1:A:77:ILE:HD11    | 14:T:6:TYR:HB3     | 1.58                     | 0.84              |
| 22:C:1031:CLA:C14  | 25:C:1054:BCR:H362 | 2.08                     | 0.84              |
| 22:C:1033:CLA:H203 | 22:C:1033:CLA:H152 | 1.59                     | 0.84              |
| 22:b:6009:CLA:CAA  | 25:h:6049:BCR:H363 | 2.08                     | 0.84              |
| 23:A:1038:PHO:H2A  | 23:A:1038:PHO:O1D  | 1.77                     | 0.84              |
| 22:B:1016:CLA:C2   | 22:H:1017:CLA:C9   | 2.56                     | 0.84              |
| 4:D:198:MET:HB3    | 22:D:1005:CLA:HED2 | 1.60                     | 0.84              |
| 2:b:5003:LEU:HB3   | 11:l:5009:PRO:O    | 1.77                     | 0.84              |
| 22:b:6011:CLA:H12  | 22:b:6013:CLA:C9   | 2.06                     | 0.84              |
| 29:c:6055:DGD:HBFI | 29:c:6055:DGD:HGB2 | 1.58                     | 0.84              |
| 23:d:6039:PHO:HMA3 | 22:d:6004:CLA:H143 | 1.57                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:k:6034:CLA:H71  | 22:k:6034:CLA:H43  | 1.56                     | 0.84              |
| 2:B:460:LEU:HD23   | 2:B:460:LEU:O      | 1.77                     | 0.84              |
| 22:B:1019:CLA:C19  | 22:B:1021:CLA:H72  | 2.07                     | 0.84              |
| 22:B:1021:CLA:HED3 | 22:B:1021:CLA:H2   | 1.60                     | 0.84              |
| 4:D:184:PHE:HE2    | 4:D:188:PHE:HD1    | 1.23                     | 0.84              |
| 24:D:1042:PQ9:H401 | 11:L:30:LEU:HD12   | 1.58                     | 0.84              |
| 11:L:24:ILE:HD13   | 12:M:18:PRO:CG     | 2.08                     | 0.84              |
| 2:b:5052:LEU:HD22  | 2:b:5311:PHE:HD1   | 1.41                     | 0.84              |
| 22:b:6009:CLA:HAA1 | 22:b:6009:CLA:HED3 | 1.35                     | 0.84              |
| 22:c:6030:CLA:HED2 | 22:c:6030:CLA:CAD  | 2.07                     | 0.84              |
| 29:c:6057:DGD:HB82 | 28:d:6059:MGE:H8B2 | 1.60                     | 0.84              |
| 22:d:6004:CLA:H201 | 28:d:6059:MGE:H8A1 | 1.58                     | 0.84              |
| 22:k:6034:CLA:C7   | 22:k:6034:CLA:H41  | 2.08                     | 0.84              |
| 13:o:5176:SER:HB3  | 13:o:5216:PHE:CE2  | 2.13                     | 0.84              |
| 1:A:116:ILE:HD11   | 1:A:158:PHE:HB3    | 1.58                     | 0.83              |
| 2:B:220:ARG:HD2    | 7:H:20:LYS:O       | 1.76                     | 0.83              |
| 2:B:463:PHE:CE1    | 22:B:1016:CLA:HBB1 | 2.12                     | 0.83              |
| 22:B:1011:CLA:H12  | 22:B:1013:CLA:C9   | 2.06                     | 0.83              |
| 22:B:1021:CLA:H41  | 28:B:1060:MGE:H242 | 1.60                     | 0.83              |
| 3:C:56:HIS:C       | 3:C:58:GLY:N       | 2.31                     | 0.83              |
| 3:C:229:ASN:HD22   | 3:C:229:ASN:N      | 1.73                     | 0.83              |
| 22:C:1033:CLA:C2   | 22:C:1033:CLA:H71  | 2.07                     | 0.83              |
| 15:U:61:VAL:HG12   | 15:U:75:LEU:HD23   | 1.58                     | 0.83              |
| 22:b:6012:CLA:CBB  | 22:b:6015:CLA:CBB  | 2.55                     | 0.83              |
| 22:c:6031:CLA:C14  | 25:c:6054:BCR:H362 | 2.08                     | 0.83              |
| 2:B:463:PHE:HE1    | 22:B:1016:CLA:HBB1 | 1.42                     | 0.83              |
| 16:V:135:GLU:O     | 16:V:139:VAL:HG23  | 1.78                     | 0.83              |
| 20:Z:23:VAL:HG13   | 20:Z:27:TYR:CE2    | 2.12                     | 0.83              |
| 1:A:160:ILE:HG21   | 3:C:431:PHE:HE1    | 1.44                     | 0.83              |
| 2:B:264:PRO:CG     | 2:B:267:LEU:HB2    | 2.09                     | 0.83              |
| 22:B:1011:CLA:HMD1 | 22:B:1013:CLA:H42  | 1.59                     | 0.83              |
| 3:c:5050:LEU:HD23  | 3:c:5051:GLY:N     | 1.91                     | 0.83              |
| 4:d:5148:ALA:HB1   | 4:d:5279:LEU:HD13  | 1.60                     | 0.83              |
| 10:k:5035:LEU:HA   | 10:k:5038:VAL:HG23 | 1.59                     | 0.83              |
| 2:B:55:MET:HE1     | 2:B:80:ILE:HD13    | 1.58                     | 0.83              |
| 7:H:6:TRP:O        | 7:H:10:ILE:HG13    | 1.79                     | 0.83              |
| 9:J:31:GLY:O       | 9:J:35:GLY:HA3     | 1.78                     | 0.83              |
| 3:c:5042:LEU:HD11  | 3:c:5049:LEU:HD13  | 1.61                     | 0.83              |
| 22:c:6027:CLA:C15  | 25:z:6053:BCR:H332 | 2.07                     | 0.83              |
| 7:h:5006:TRP:O     | 7:h:5010:ILE:HG13  | 1.79                     | 0.83              |
| 10:k:5011:LEU:HD11 | 10:k:5022:VAL:HG21 | 1.58                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:t:5001:MET:O    | 14:t:5004:ILE:HG23 | 1.77                     | 0.83              |
| 1:A:301:ASN:HD22   | 3:C:407:VAL:HG11   | 1.41                     | 0.83              |
| 22:B:1009:CLA:CAA  | 25:H:1049:BCR:H363 | 2.08                     | 0.83              |
| 25:B:1047:BCR:H403 | 25:B:1047:BCR:H372 | 1.56                     | 0.83              |
| 13:O:176:SER:HB3   | 13:O:216:PHE:CE2   | 2.13                     | 0.83              |
| 14:T:1:MET:O       | 14:T:4:ILE:HG23    | 1.77                     | 0.83              |
| 1:a:5278:TRP:CE3   | 1:a:5278:TRP:HA    | 2.13                     | 0.83              |
| 22:d:6008:CLA:HMC3 | 22:d:6008:CLA:HBC2 | 1.60                     | 0.83              |
| 9:j:5031:GLY:O     | 9:j:5035:GLY:HA3   | 1.78                     | 0.83              |
| 26:A:1063:LHG:H161 | 26:A:1063:LHG:C12  | 2.05                     | 0.83              |
| 22:B:1022:CLA:H142 | 22:B:1022:CLA:C6   | 1.98                     | 0.83              |
| 3:C:42:LEU:CD1     | 3:C:49:LEU:HD11    | 2.09                     | 0.83              |
| 23:D:1039:PHO:HBC2 | 23:D:1039:PHO:CHD  | 2.06                     | 0.83              |
| 22:K:1034:CLA:C7   | 22:K:1034:CLA:H41  | 2.08                     | 0.83              |
| 1:a:5103:ASP:HA    | 1:a:5106:LEU:HD12  | 1.58                     | 0.83              |
| 22:b:6019:CLA:HBA1 | 22:b:6019:CLA:CHA  | 2.07                     | 0.83              |
| 11:l:5024:ILE:HD13 | 12:m:5018:PRO:CG   | 2.08                     | 0.83              |
| 24:D:1042:PQ9:H392 | 28:L:1061:MGE:H241 | 1.58                     | 0.83              |
| 2:b:5264:PRO:CG    | 2:b:5267:LEU:HB2   | 2.09                     | 0.83              |
| 22:b:6011:CLA:CAD  | 22:b:6013:CLA:C1   | 2.57                     | 0.83              |
| 3:c:5318:LEU:CD2   | 3:c:5328:VAL:HG11  | 2.09                     | 0.83              |
| 24:d:6042:PQ9:H401 | 11:l:5030:LEU:HD12 | 1.58                     | 0.83              |
| 23:A:1038:PHO:H202 | 22:D:1005:CLA:CMB  | 2.08                     | 0.83              |
| 22:C:1027:CLA:C15  | 25:Z:1053:BCR:H332 | 2.07                     | 0.83              |
| 22:C:1032:CLA:C15  | 10:K:33:PHE:CZ     | 2.48                     | 0.83              |
| 9:J:21:VAL:CG1     | 9:J:22:ILE:HD12    | 2.09                     | 0.83              |
| 28:b:6060:MGE:C3B  | 28:b:6060:MGE:C7B  | 2.57                     | 0.83              |
| 22:c:6033:CLA:H203 | 22:c:6033:CLA:H152 | 1.59                     | 0.83              |
| 28:d:6059:MGE:H251 | 28:d:6059:MGE:H212 | 1.56                     | 0.83              |
| 10:k:5033:PHE:HD1  | 10:k:5033:PHE:O    | 1.62                     | 0.83              |
| 14:t:5018:PHE:HA   | 25:t:1046:BCR:C33  | 2.08                     | 0.83              |
| 1:A:184:ILE:HG12   | 4:D:186:GLN:HE21   | 1.44                     | 0.83              |
| 2:B:7:ARG:HH11     | 2:B:7:ARG:CG       | 1.91                     | 0.83              |
| 22:B:1022:CLA:C6   | 22:B:1022:CLA:H143 | 2.09                     | 0.83              |
| 3:C:185:LEU:HD12   | 3:C:230:LEU:HD22   | 1.59                     | 0.83              |
| 22:C:1025:CLA:H141 | 22:C:1031:CLA:CMB  | 2.05                     | 0.83              |
| 14:T:4:ILE:HD13    | 14:T:5:THR:H       | 1.40                     | 0.83              |
| 1:a:5291:SER:HB3   | 3:c:5431:PHE:CE1   | 2.13                     | 0.83              |
| 3:c:5185:LEU:HD12  | 3:c:5230:LEU:HD22  | 1.59                     | 0.83              |
| 22:D:1008:CLA:C14  | 22:D:1008:CLA:H18  | 2.07                     | 0.83              |
| 1:a:5317:TRP:N     | 4:d:5063:LEU:HD21  | 1.94                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:z:5028:ALA:O    | 20:z:5030:PRO:HD3  | 1.79                     | 0.83              |
| 1:A:278:TRP:CE3    | 1:A:278:TRP:HA     | 2.13                     | 0.82              |
| 3:C:318:LEU:CD2    | 3:C:328:VAL:HG11   | 2.08                     | 0.82              |
| 25:h:6049:BCR:H23C | 25:h:6049:BCR:H392 | 0.83                     | 0.82              |
| 3:C:429:SER:O      | 3:C:432:VAL:HG12   | 1.80                     | 0.82              |
| 4:D:58:TRP:HE1     | 5:E:64:PRO:HD2     | 1.45                     | 0.82              |
| 25:H:1049:BCR:H23C | 25:H:1049:BCR:H392 | 0.83                     | 0.82              |
| 14:T:23:PHE:CZ     | 2:b:5112:CYS:SG    | 2.72                     | 0.82              |
| 22:b:6016:CLA:C2   | 22:h:6017:CLA:C9   | 2.56                     | 0.82              |
| 3:c:5056:HIS:C     | 3:c:5058:GLY:N     | 2.31                     | 0.82              |
| 1:A:58:VAL:HG12    | 1:A:60:ILE:H       | 1.42                     | 0.82              |
| 26:A:1063:LHG:H291 | 22:C:1032:CLA:H71  | 1.60                     | 0.82              |
| 22:D:1008:CLA:H193 | 22:D:1008:CLA:H141 | 1.60                     | 0.82              |
| 4:d:5198:MET:CB    | 22:d:6005:CLA:HED2 | 2.10                     | 0.82              |
| 2:B:36:SER:CB      | 25:t:1046:BCR:H401 | 2.09                     | 0.82              |
| 4:D:148:ALA:HB1    | 4:D:279:LEU:HD13   | 1.60                     | 0.82              |
| 10:K:28:ILE:HD13   | 10:K:31:LEU:HD12   | 1.60                     | 0.82              |
| 14:T:21:ILE:HD12   | 25:T:6046:BCR:HC42 | 1.61                     | 0.82              |
| 2:b:5488:PRO:O     | 2:b:5489:GLU:HB3   | 1.78                     | 0.82              |
| 22:c:6029:CLA:HMD1 | 22:c:6031:CLA:HAB  | 1.59                     | 0.82              |
| 22:d:6008:CLA:H193 | 22:d:6008:CLA:H141 | 1.60                     | 0.82              |
| 1:A:149:ALA:HB3    | 1:A:150:PRO:HD3    | 1.58                     | 0.82              |
| 22:B:1011:CLA:CAD  | 22:B:1013:CLA:C1   | 2.57                     | 0.82              |
| 22:C:1033:CLA:C2   | 22:C:1033:CLA:C7   | 2.54                     | 0.82              |
| 31:F:1040:HEM:HMB2 | 31:F:1040:HEM:HBB2 | 1.58                     | 0.82              |
| 22:a:6003:CLA:C14  | 23:a:6038:PHO:C8   | 2.58                     | 0.82              |
| 2:b:5012:LEU:HD13  | 22:b:6020:CLA:HMC2 | 1.62                     | 0.82              |
| 2:b:5224:ARG:HG2   | 7:h:5025:TRP:NE1   | 1.95                     | 0.82              |
| 22:b:6009:CLA:C14  | 22:b:6009:CLA:C10  | 2.55                     | 0.82              |
| 3:C:49:LEU:CD1     | 3:C:49:LEU:H       | 1.91                     | 0.82              |
| 3:C:315:MET:HE3    | 3:C:315:MET:HA     | 1.61                     | 0.82              |
| 29:C:1056:DGD:C6D  | 29:C:1056:DGD:C5E  | 2.50                     | 0.82              |
| 1:a:5223:LEU:HD21  | 4:d:5265:ARG:HG2   | 1.62                     | 0.82              |
| 4:d:5198:MET:HB3   | 22:d:6005:CLA:HED2 | 1.60                     | 0.82              |
| 3:C:89:ILE:HG12    | 3:C:111:PHE:HD2    | 1.45                     | 0.82              |
| 2:b:5012:LEU:HD22  | 2:b:5019:LEU:HD13  | 1.61                     | 0.82              |
| 22:b:6022:CLA:HHD  | 22:b:6022:CLA:CBC  | 2.09                     | 0.82              |
| 22:c:6031:CLA:OBD  | 22:c:6033:CLA:C12  | 2.28                     | 0.82              |
| 1:A:279:ARG:HB3    | 4:D:212:ALA:HB2    | 1.60                     | 0.82              |
| 23:A:1038:PHO:HBC3 | 23:A:1038:PHO:CHD  | 2.10                     | 0.82              |
| 2:B:224:ARG:HG2    | 7:H:25:TRP:NE1     | 1.95                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:301:ALA:O      | 2:B:304:ALA:HB3    | 1.80                     | 0.82              |
| 12:M:9:ILE:HD11    | 12:m:5009:ILE:CD1  | 2.10                     | 0.82              |
| 2:b:5007:ARG:HH11  | 2:b:5007:ARG:CG    | 1.91                     | 0.82              |
| 10:k:5028:ILE:HD13 | 10:k:5031:LEU:HD12 | 1.60                     | 0.82              |
| 16:v:5135:GLU:O    | 16:v:5139:VAL:HG23 | 1.79                     | 0.82              |
| 2:B:80:ILE:HD11    | 2:B:93:PHE:HZ      | 1.45                     | 0.82              |
| 13:O:45:CYS:HB2    | 13:O:46:PRO:HD2    | 1.62                     | 0.82              |
| 22:c:6033:CLA:H91  | 22:c:6036:CLA:HAA1 | 1.62                     | 0.82              |
| 29:c:6055:DGD:HB21 | 29:c:6055:DGD:HA21 | 1.62                     | 0.82              |
| 22:A:1003:CLA:C14  | 23:A:1038:PHO:C8   | 2.58                     | 0.82              |
| 22:A:1007:CLA:H42  | 22:C:1029:CLA:H191 | 1.60                     | 0.82              |
| 2:B:12:LEU:HD13    | 22:B:1020:CLA:HMC2 | 1.62                     | 0.82              |
| 2:B:12:LEU:HD22    | 2:B:19:LEU:HD13    | 1.61                     | 0.82              |
| 3:C:117:VAL:CG1    | 3:C:118:HIS:N      | 2.43                     | 0.82              |
| 1:a:5216:GLY:HA2   | 4:d:5268:HIS:O     | 1.80                     | 0.82              |
| 22:b:6022:CLA:C6   | 22:b:6022:CLA:H143 | 2.09                     | 0.82              |
| 9:j:5021:VAL:CG1   | 9:j:5022:ILE:HD12  | 2.09                     | 0.82              |
| 22:A:1006:CLA:H172 | 25:D:1050:BCR:H272 | 1.62                     | 0.81              |
| 22:B:1009:CLA:CED  | 22:B:1009:CLA:C2A  | 2.53                     | 0.81              |
| 2:b:5359:MET:HG3   | 2:b:5359:MET:O     | 1.78                     | 0.81              |
| 22:c:6030:CLA:CBC  | 22:c:6030:CLA:CHD  | 2.58                     | 0.81              |
| 22:d:6008:CLA:C14  | 22:d:6008:CLA:H18  | 2.07                     | 0.81              |
| 10:k:5031:LEU:O    | 10:k:5034:ALA:HB3  | 1.81                     | 0.81              |
| 1:A:120:LEU:HD21   | 1:A:155:PHE:HA     | 1.62                     | 0.81              |
| 3:C:92:ILE:H       | 3:C:92:ILE:HD12    | 1.44                     | 0.81              |
| 3:C:263:ALA:CB     | 3:C:264:PHE:HE2    | 1.93                     | 0.81              |
| 4:D:36:LEU:HD23    | 4:D:37:LEU:N       | 1.95                     | 0.81              |
| 13:O:83:LYS:HE3    | 2:b:5049:ASP:CB    | 2.09                     | 0.81              |
| 2:b:5298:LEU:O     | 2:b:5301:ALA:HB3   | 1.80                     | 0.81              |
| 22:b:6009:CLA:C8   | 22:b:6009:CLA:H142 | 2.09                     | 0.81              |
| 22:b:6011:CLA:HED2 | 22:b:6012:CLA:HED2 | 1.61                     | 0.81              |
| 22:b:6021:CLA:HED3 | 22:b:6021:CLA:H2   | 1.60                     | 0.81              |
| 22:b:6023:CLA:H152 | 22:b:6024:CLA:CHB  | 2.10                     | 0.81              |
| 25:b:6045:BCR:H383 | 25:b:6045:BCR:C23  | 2.09                     | 0.81              |
| 3:c:5049:LEU:HD22  | 3:c:5052:ALA:CB    | 2.10                     | 0.81              |
| 14:t:5004:ILE:HD13 | 14:t:5005:THR:H    | 1.40                     | 0.81              |
| 2:B:488:PRO:O      | 2:B:489:GLU:HB3    | 1.78                     | 0.81              |
| 22:B:1023:CLA:H152 | 22:B:1024:CLA:CHB  | 2.10                     | 0.81              |
| 28:B:1060:MGE:C3B  | 28:B:1060:MGE:C7B  | 2.57                     | 0.81              |
| 3:C:48:LYS:HG3     | 3:C:49:LEU:HD12    | 1.62                     | 0.81              |
| 3:C:128:GLY:HA3    | 22:C:1037:CLA:HAC2 | 1.61                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5337:HIS:O     | 4:d:5351:ALA:CB    | 2.29                     | 0.81              |
| 22:a:6007:CLA:H42  | 22:c:6029:CLA:H191 | 1.60                     | 0.81              |
| 22:b:6009:CLA:HMB3 | 25:h:6049:BCR:C27  | 1.98                     | 0.81              |
| 3:c:5107:ASP:HB3   | 3:c:5110:PRO:CD    | 2.10                     | 0.81              |
| 3:c:5117:VAL:CG1   | 3:c:5118:HIS:N     | 2.43                     | 0.81              |
| 3:c:5315:MET:HA    | 3:c:5315:MET:HE3   | 1.61                     | 0.81              |
| 22:c:6031:CLA:H141 | 25:c:6054:BCR:C36  | 2.10                     | 0.81              |
| 29:c:6056:DGD:C9B  | 29:c:6056:DGD:HBF1 | 2.11                     | 0.81              |
| 4:d:5036:LEU:HD23  | 4:d:5037:LEU:N     | 1.95                     | 0.81              |
| 2:B:359:MET:HG3    | 2:B:359:MET:O      | 1.78                     | 0.81              |
| 22:D:1008:CLA:HMC3 | 22:D:1008:CLA:HBC2 | 1.60                     | 0.81              |
| 22:K:1034:CLA:H143 | 22:K:1034:CLA:C10  | 2.06                     | 0.81              |
| 13:O:141:ARG:HG2   | 13:O:141:ARG:HH11  | 1.44                     | 0.81              |
| 1:a:5120:LEU:HD21  | 1:a:5155:PHE:HA    | 1.62                     | 0.81              |
| 23:a:6038:PHO:HBC3 | 23:a:6038:PHO:HHD  | 1.62                     | 0.81              |
| 3:c:5092:ILE:H     | 3:c:5092:ILE:HD12  | 1.44                     | 0.81              |
| 3:c:5333:GLY:N     | 3:c:5338:GLY:HA2   | 1.96                     | 0.81              |
| 22:d:6008:CLA:C14  | 22:d:6008:CLA:C17  | 2.59                     | 0.81              |
| 13:o:5045:CYS:HB2  | 13:o:5046:PRO:HD2  | 1.62                     | 0.81              |
| 13:o:5223:ILE:HG22 | 13:o:5243:SER:HB3  | 1.62                     | 0.81              |
| 4:D:198:MET:CB     | 22:D:1005:CLA:HED2 | 2.10                     | 0.81              |
| 11:L:8:GLN:NE2     | 11:L:8:GLN:H       | 1.78                     | 0.81              |
| 1:a:5259:ILE:N     | 4:d:5128:ARG:HH22  | 1.79                     | 0.81              |
| 22:b:6012:CLA:HHD  | 22:b:6012:CLA:HBC3 | 1.60                     | 0.81              |
| 22:c:6027:CLA:H121 | 22:c:6027:CLA:C18  | 2.11                     | 0.81              |
| 22:c:6033:CLA:C2   | 22:c:6033:CLA:H71  | 2.07                     | 0.81              |
| 25:k:6052:BCR:H383 | 25:k:6052:BCR:H372 | 1.62                     | 0.81              |
| 13:o:5172:PHE:CD1  | 13:o:5221:GLY:HA3  | 2.15                     | 0.81              |
| 1:A:259:ILE:N      | 4:D:128:ARG:HH22   | 1.79                     | 0.81              |
| 2:B:174:LEU:HD23   | 2:B:266:GLU:CG     | 2.10                     | 0.81              |
| 2:B:298:LEU:O      | 2:B:301:ALA:HB3    | 1.80                     | 0.81              |
| 22:B:1012:CLA:HBC3 | 22:B:1012:CLA:HHD  | 1.60                     | 0.81              |
| 2:b:5125:ASP:OD2   | 7:h:5018:TYR:HB2   | 1.81                     | 0.81              |
| 3:c:5141:GLU:O     | 3:c:5144:SER:HB2   | 1.81                     | 0.81              |
| 4:d:5139:ARG:NH1   | 4:d:5265:ARG:NH2   | 2.28                     | 0.81              |
| 3:C:293:ASN:HD21   | 3:C:295:THR:HB     | 1.44                     | 0.81              |
| 24:D:1042:PQ9:H342 | 24:D:1042:PQ9:C30  | 2.10                     | 0.81              |
| 13:O:172:PHE:CD1   | 13:O:221:GLY:HA3   | 2.14                     | 0.81              |
| 25:T:6046:BCR:H401 | 2:b:5036:SER:CB    | 2.09                     | 0.81              |
| 1:a:5184:ILE:HG12  | 4:d:5186:GLN:HE21  | 1.44                     | 0.81              |
| 22:a:6003:CLA:CED  | 22:a:6003:CLA:H2A  | 2.11                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:d:6042:PQ9:H342 | 24:d:6042:PQ9:C30  | 2.10                     | 0.81              |
| 25:h:6049:BCR:H292 | 17:x:5016:LEU:HD11 | 1.63                     | 0.81              |
| 11:l:5008:GLN:NE2  | 11:l:5008:GLN:H    | 1.78                     | 0.81              |
| 22:A:1006:CLA:CBC  | 4:D:182:LEU:HD21   | 2.11                     | 0.81              |
| 22:B:1011:CLA:C2D  | 22:B:1013:CLA:C4   | 2.59                     | 0.81              |
| 3:C:49:LEU:HD22    | 3:C:52:ALA:CB      | 2.10                     | 0.81              |
| 22:D:1008:CLA:C14  | 22:D:1008:CLA:C17  | 2.59                     | 0.81              |
| 22:a:6006:CLA:C16  | 25:d:6050:BCR:H272 | 2.11                     | 0.81              |
| 2:b:5174:LEU:HD23  | 2:b:5266:GLU:CG    | 2.10                     | 0.81              |
| 3:c:5293:ASN:HD21  | 3:c:5295:THR:HB    | 1.44                     | 0.81              |
| 4:d:5058:TRP:HE1   | 5:e:5064:PRO:HD2   | 1.45                     | 0.81              |
| 1:A:317:TRP:N      | 4:D:63:LEU:HD21    | 1.94                     | 0.81              |
| 22:B:1009:CLA:C14  | 22:B:1009:CLA:C10  | 2.55                     | 0.81              |
| 22:B:1010:CLA:H12  | 22:B:1010:CLA:CBD  | 2.11                     | 0.81              |
| 25:C:1054:BCR:C40  | 25:C:1054:BCR:C23  | 2.30                     | 0.81              |
| 10:K:31:LEU:HB3    | 25:K:1051:BCR:H14C | 1.63                     | 0.81              |
| 13:O:223:ILE:HG22  | 13:O:243:SER:HB3   | 1.62                     | 0.81              |
| 20:Z:28:ALA:O      | 20:Z:30:PRO:HD3    | 1.79                     | 0.81              |
| 1:a:5129:ARG:CZ    | 4:d:5256:ILE:HD12  | 2.11                     | 0.81              |
| 22:b:6022:CLA:CGA  | 22:b:6022:CLA:C4   | 2.59                     | 0.81              |
| 22:b:6023:CLA:C13  | 22:b:6024:CLA:CMA  | 2.56                     | 0.81              |
| 3:c:5128:GLY:HA3   | 22:c:6037:CLA:HAC2 | 1.61                     | 0.81              |
| 3:c:5305:THR:HG22  | 3:c:5308:GLU:HB2   | 1.62                     | 0.81              |
| 3:c:5428:THR:HG23  | 3:c:5429:SER:N     | 1.94                     | 0.81              |
| 24:d:6042:PQ9:H301 | 24:d:6042:PQ9:C34  | 2.06                     | 0.81              |
| 1:A:278:TRP:HA     | 1:A:278:TRP:HE3    | 1.46                     | 0.81              |
| 3:C:333:GLY:N      | 3:C:338:GLY:HA2    | 1.96                     | 0.81              |
| 22:C:1033:CLA:H91  | 22:C:1036:CLA:HAA1 | 1.62                     | 0.81              |
| 29:C:1056:DGD:C9B  | 29:C:1056:DGD:HBf1 | 2.11                     | 0.81              |
| 4:d:5120:PHE:HA    | 4:d:5123:ILE:HD12  | 1.62                     | 0.81              |
| 25:k:6052:BCR:H371 | 25:k:6052:BCR:C27  | 2.09                     | 0.81              |
| 1:A:196:PRO:HA     | 1:A:199:GLN:HG3    | 1.62                     | 0.80              |
| 2:B:103:LEU:CB     | 22:B:1014:CLA:H92  | 2.12                     | 0.80              |
| 2:B:115:TRP:O      | 2:B:118:TRP:HB3    | 1.81                     | 0.80              |
| 2:B:264:PRO:HG2    | 2:B:267:LEU:HB2    | 1.63                     | 0.80              |
| 2:B:362:PHE:CZ     | 27:D:1068:IOD:I    | 3.04                     | 0.80              |
| 3:C:185:LEU:HG     | 3:C:199:ILE:HD11   | 1.63                     | 0.80              |
| 3:C:428:THR:HG23   | 3:C:429:SER:H      | 1.46                     | 0.80              |
| 3:C:428:THR:HG23   | 3:C:429:SER:N      | 1.94                     | 0.80              |
| 2:b:5098:LEU:HD13  | 2:b:5098:LEU:O     | 1.81                     | 0.80              |
| 3:c:5263:ALA:CB    | 3:c:5264:PHE:HE2   | 1.93                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:c:6054:BCR:H23C | 25:c:6054:BCR:H403 | 0.82                     | 0.80              |
| 13:o:5141:ARG:HG2  | 13:o:5141:ARG:HH11 | 1.44                     | 0.80              |
| 1:A:16:ARG:HA      | 1:A:19:ASN:HD21    | 1.46                     | 0.80              |
| 22:A:1006:CLA:C16  | 25:D:1050:BCR:H272 | 2.11                     | 0.80              |
| 25:A:1044:BCR:H371 | 25:A:1044:BCR:H403 | 1.31                     | 0.80              |
| 22:B:1023:CLA:C13  | 22:B:1024:CLA:CMA  | 2.56                     | 0.80              |
| 1:a:5160:ILE:HG21  | 3:c:5431:PHE:HE1   | 1.44                     | 0.80              |
| 17:x:5043:ILE:HG22 | 17:x:5043:ILE:O    | 1.80                     | 0.80              |
| 1:A:129:ARG:CZ     | 4:D:256:ILE:HD12   | 2.11                     | 0.80              |
| 3:C:397:THR:OG1    | 3:C:398:HIS:N      | 2.13                     | 0.80              |
| 22:C:1035:CLA:CBB  | 22:K:1034:CLA:HMA2 | 2.11                     | 0.80              |
| 24:a:6043:PQ9:C45  | 28:d:6059:MGE:CAA  | 2.57                     | 0.80              |
| 22:c:6035:CLA:CBB  | 22:k:6034:CLA:HMA2 | 2.11                     | 0.80              |
| 29:c:6057:DGD:HBG2 | 29:c:6057:DGD:CEB  | 2.10                     | 0.80              |
| 15:u:5083:THR:HG22 | 15:u:5084:VAL:H    | 1.47                     | 0.80              |
| 2:B:98:LEU:O       | 2:B:98:LEU:HD13    | 1.81                     | 0.80              |
| 29:C:1055:DGD:HB21 | 29:C:1055:DGD:HA21 | 1.62                     | 0.80              |
| 22:b:6009:CLA:H8   | 22:b:6009:CLA:H142 | 1.62                     | 0.80              |
| 22:b:6021:CLA:H41  | 28:b:6060:MGE:H242 | 1.60                     | 0.80              |
| 23:A:1038:PHO:HBC3 | 23:A:1038:PHO:HHD  | 1.62                     | 0.80              |
| 2:B:332:LYS:HB3    | 2:B:444:ARG:NH1    | 1.96                     | 0.80              |
| 3:C:107:ASP:HB3    | 3:C:110:PRO:CD     | 2.10                     | 0.80              |
| 3:C:141:GLU:O      | 3:C:144:SER:HB2    | 1.81                     | 0.80              |
| 29:C:1056:DGD:HAV1 | 29:C:1057:DGD:HA82 | 1.64                     | 0.80              |
| 7:H:38:PHE:HB2     | 25:H:1049:BCR:H10C | 1.64                     | 0.80              |
| 22:a:6006:CLA:H172 | 25:d:6050:BCR:H272 | 1.62                     | 0.80              |
| 2:b:5005:TRP:CA    | 2:b:5008:VAL:HG13  | 2.11                     | 0.80              |
| 2:b:5099:ALA:HB1   | 22:b:6014:CLA:H42  | 1.64                     | 0.80              |
| 3:c:5429:SER:O     | 3:c:5432:VAL:HG12  | 1.80                     | 0.80              |
| 22:B:1009:CLA:C1A  | 22:B:1009:CLA:O1A  | 2.30                     | 0.80              |
| 25:B:1045:BCR:H23C | 25:B:1045:BCR:C38  | 2.06                     | 0.80              |
| 3:C:49:LEU:HD11    | 22:C:1035:CLA:CMA  | 2.11                     | 0.80              |
| 22:C:1029:CLA:O1A  | 22:C:1029:CLA:CHA  | 2.30                     | 0.80              |
| 2:b:5115:TRP:O     | 2:b:5118:TRP:HB3   | 1.81                     | 0.80              |
| 22:b:6022:CLA:O1D  | 22:b:6022:CLA:CGA  | 2.30                     | 0.80              |
| 3:c:5049:LEU:HD11  | 22:c:6035:CLA:CMA  | 2.11                     | 0.80              |
| 3:c:5128:GLY:CA    | 22:c:6037:CLA:HAC2 | 2.12                     | 0.80              |
| 7:h:5030:LEU:HD12  | 7:h:5033:VAL:HG21  | 1.64                     | 0.80              |
| 22:A:1003:CLA:CED  | 22:A:1003:CLA:H2A  | 2.11                     | 0.80              |
| 29:B:1058:DGD:C6B  | 29:B:1058:DGD:CAB  | 2.55                     | 0.80              |
| 22:C:1025:CLA:HHB  | 22:C:1025:CLA:C1   | 2.06                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1029:CLA:H43  | 25:C:1054:BCR:H321 | 1.63                     | 0.80              |
| 22:C:1033:CLA:CMA  | 22:K:1034:CLA:CAC  | 2.60                     | 0.80              |
| 2:b:5103:LEU:CB    | 22:b:6014:CLA:H92  | 2.11                     | 0.80              |
| 3:c:5042:LEU:HD11  | 3:c:5049:LEU:HD11  | 1.64                     | 0.80              |
| 22:c:6033:CLA:CMA  | 22:k:6034:CLA:CAC  | 2.60                     | 0.80              |
| 29:c:6055:DGD:CIB  | 29:c:6055:DGD:CEB  | 2.58                     | 0.80              |
| 2:B:314:TYR:CE2    | 2:B:316:GLY:HA3    | 2.17                     | 0.80              |
| 22:C:1031:CLA:H141 | 25:C:1054:BCR:C36  | 2.10                     | 0.80              |
| 25:C:1052:BCR:H371 | 25:C:1052:BCR:C27  | 2.09                     | 0.80              |
| 1:a:5216:GLY:CA    | 4:d:5268:HIS:O     | 2.29                     | 0.80              |
| 1:a:5325:ASN:HA    | 1:a:5328:MET:HE3   | 1.62                     | 0.80              |
| 22:b:6012:CLA:C1D  | 22:b:6020:CLA:H202 | 2.12                     | 0.80              |
| 22:b:6022:CLA:C4D  | 22:b:6022:CLA:C1   | 2.60                     | 0.80              |
| 1:A:325:ASN:HA     | 1:A:328:MET:HE3    | 1.62                     | 0.80              |
| 22:C:1027:CLA:H121 | 22:C:1027:CLA:C18  | 2.11                     | 0.80              |
| 29:C:1057:DGD:HB82 | 28:D:1059:MGE:H8B2 | 1.60                     | 0.80              |
| 22:a:6006:CLA:CBC  | 4:d:5182:LEU:HD21  | 2.11                     | 0.80              |
| 22:b:6010:CLA:H151 | 29:b:6058:DGD:HA82 | 1.64                     | 0.80              |
| 29:c:6056:DGD:HAV1 | 29:c:6057:DGD:HA82 | 1.64                     | 0.80              |
| 4:d:5153:PHE:HB2   | 22:d:6004:CLA:H41  | 1.64                     | 0.80              |
| 16:v:5045:ILE:HD12 | 16:v:5045:ILE:N    | 1.96                     | 0.80              |
| 22:B:1022:CLA:CGA  | 22:B:1022:CLA:C4   | 2.59                     | 0.80              |
| 3:C:396:MET:HE1    | 16:V:74:THR:HA     | 1.63                     | 0.80              |
| 4:D:88:SER:HA      | 7:H:50:ASN:ND2     | 1.93                     | 0.80              |
| 13:O:141:ARG:HG2   | 13:O:141:ARG:NH1   | 1.96                     | 0.80              |
| 23:a:6038:PHO:C9   | 22:d:6005:CLA:H18  | 2.11                     | 0.80              |
| 2:b:5172:TYR:O     | 2:b:5174:LEU:CA    | 2.29                     | 0.80              |
| 2:b:5468:TRP:HE1   | 22:b:6019:CLA:HED2 | 1.47                     | 0.80              |
| 3:c:5048:LYS:HG3   | 3:c:5049:LEU:HD12  | 1.62                     | 0.80              |
| 3:c:5307:PRO:HA    | 3:c:5358:PHE:CD1   | 2.17                     | 0.80              |
| 22:c:6025:CLA:C2B  | 22:c:6025:CLA:H43  | 2.11                     | 0.80              |
| 13:o:5243:SER:OG   | 13:o:5261:ILE:HB   | 1.82                     | 0.80              |
| 22:B:1016:CLA:CHA  | 22:B:1016:CLA:O1A  | 2.30                     | 0.79              |
| 3:C:128:GLY:CA     | 22:C:1037:CLA:HAC2 | 2.12                     | 0.79              |
| 4:D:120:PHE:HA     | 4:D:123:ILE:HD12   | 1.62                     | 0.79              |
| 5:E:13:ILE:HA      | 5:E:16:SER:HB2     | 1.64                     | 0.79              |
| 7:H:43:LEU:HD21    | 17:X:19:PHE:CZ     | 2.16                     | 0.79              |
| 15:U:28:ASN:HD22   | 15:U:54:PRO:HB2    | 1.46                     | 0.79              |
| 16:V:45:ILE:HD12   | 16:V:45:ILE:N      | 1.96                     | 0.79              |
| 1:a:5196:PRO:HA    | 1:a:5199:GLN:HG3   | 1.62                     | 0.79              |
| 3:c:5089:ILE:HG12  | 3:c:5111:PHE:HD2   | 1.45                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:5:TRP:CA       | 2:B:8:VAL:HG13     | 2.11                     | 0.79              |
| 22:B:1011:CLA:O1A  | 22:B:1011:CLA:C4   | 2.30                     | 0.79              |
| 22:B:1022:CLA:C4D  | 22:B:1022:CLA:C1   | 2.60                     | 0.79              |
| 25:B:1045:BCR:H383 | 25:B:1045:BCR:C23  | 2.09                     | 0.79              |
| 25:H:1049:BCR:H292 | 17:X:16:LEU:HD11   | 1.63                     | 0.79              |
| 15:U:68:THR:HG23   | 15:U:70:ARG:H      | 1.45                     | 0.79              |
| 1:a:5314:ILE:HD12  | 4:d:5058:TRP:CZ3   | 2.17                     | 0.79              |
| 22:a:6006:CLA:H161 | 25:d:6050:BCR:H272 | 1.64                     | 0.79              |
| 2:b:5105:GLY:HA2   | 25:b:6047:BCR:H402 | 1.64                     | 0.79              |
| 2:b:5264:PRO:HG2   | 2:b:5267:LEU:HB2   | 1.63                     | 0.79              |
| 22:b:6022:CLA:O1A  | 22:b:6022:CLA:C4   | 2.30                     | 0.79              |
| 22:b:6023:CLA:C9   | 22:b:6024:CLA:H151 | 2.12                     | 0.79              |
| 29:b:6058:DGD:C6B  | 29:b:6058:DGD:CAB  | 2.55                     | 0.79              |
| 22:c:6025:CLA:H151 | 22:c:6031:CLA:H91  | 1.64                     | 0.79              |
| 5:e:5013:ILE:HA    | 5:e:5016:SER:HB2   | 1.64                     | 0.79              |
| 15:u:5068:THR:HG23 | 15:u:5070:ARG:H    | 1.45                     | 0.79              |
| 29:C:1055:DGD:CIB  | 29:C:1055:DGD:CEB  | 2.58                     | 0.79              |
| 18:Y:43:ARG:CD     | 18:Y:44:GLY:H      | 1.95                     | 0.79              |
| 3:c:5396:MET:HE1   | 16:v:5074:THR:HA   | 1.63                     | 0.79              |
| 4:d:5057:SER:CB    | 4:d:5079:SER:HB3   | 2.13                     | 0.79              |
| 11:l:5021:LEU:HB2  | 14:t:5016:LEU:HD21 | 1.64                     | 0.79              |
| 13:o:5179:THR:HG22 | 13:o:5180:ALA:N    | 1.92                     | 0.79              |
| 1:A:314:ILE:HD12   | 4:D:58:TRP:CZ3     | 2.17                     | 0.79              |
| 22:B:1022:CLA:O1D  | 22:B:1022:CLA:CGA  | 2.30                     | 0.79              |
| 22:B:1022:CLA:O1A  | 22:B:1022:CLA:C4   | 2.30                     | 0.79              |
| 22:C:1030:CLA:H172 | 22:C:1030:CLA:H122 | 1.62                     | 0.79              |
| 25:C:1052:BCR:H383 | 25:C:1052:BCR:H372 | 1.61                     | 0.79              |
| 7:H:30:LEU:HD12    | 7:H:33:VAL:HG21    | 1.64                     | 0.79              |
| 20:Z:55:GLY:HA2    | 25:Z:1053:BCR:H311 | 1.65                     | 0.79              |
| 1:a:5279:ARG:HB3   | 4:d:5212:ALA:HB2   | 1.64                     | 0.79              |
| 2:b:5301:ALA:O     | 2:b:5304:ALA:HB3   | 1.80                     | 0.79              |
| 22:b:6011:CLA:C2D  | 22:b:6013:CLA:C4   | 2.59                     | 0.79              |
| 3:c:5161:LEU:HD23  | 3:c:5162:GLY:N     | 1.96                     | 0.79              |
| 22:c:6029:CLA:CHA  | 22:c:6029:CLA:O1A  | 2.30                     | 0.79              |
| 1:A:223:LEU:HD21   | 4:D:265:ARG:HG2    | 1.62                     | 0.79              |
| 3:C:50:LEU:HD21    | 3:C:54:VAL:HG21    | 1.65                     | 0.79              |
| 3:C:292:PHE:CD1    | 29:C:1055:DGD:HD1  | 2.18                     | 0.79              |
| 3:C:305:THR:HG22   | 3:C:308:GLU:HB2    | 1.62                     | 0.79              |
| 4:D:146:PHE:O      | 4:D:149:PRO:HD2    | 1.82                     | 0.79              |
| 11:L:36:PHE:CE1    | 12:M:7:GLY:HA3     | 2.18                     | 0.79              |
| 13:O:31:LEU:HD13   | 13:O:36:ILE:HD11   | 1.64                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:U:83:THR:HG22   | 15:U:84:VAL:H      | 1.47                     | 0.79              |
| 25:b:6047:BCR:C12  | 25:b:6047:BCR:H341 | 2.12                     | 0.79              |
| 3:c:5220:GLY:O     | 3:c:5221:GLU:HG3   | 1.81                     | 0.79              |
| 22:c:6031:CLA:HBC2 | 22:c:6031:CLA:CHD  | 2.11                     | 0.79              |
| 11:l:5036:PHE:CE1  | 12:m:5007:GLY:HA3  | 2.18                     | 0.79              |
| 1:A:224:ILE:HA     | 2:B:482:ILE:HG12   | 1.64                     | 0.79              |
| 1:A:270:SER:HA     | 4:D:232:PHE:CZ     | 2.17                     | 0.79              |
| 3:C:161:LEU:HD23   | 3:C:162:GLY:N      | 1.96                     | 0.79              |
| 22:C:1025:CLA:C2B  | 22:C:1025:CLA:H43  | 2.11                     | 0.79              |
| 26:a:6063:LHG:H291 | 22:c:6032:CLA:H71  | 1.64                     | 0.79              |
| 22:b:6024:CLA:O2A  | 22:b:6024:CLA:H2A  | 1.83                     | 0.79              |
| 22:c:6028:CLA:H91  | 29:c:6056:DGD:HBT1 | 1.65                     | 0.79              |
| 4:d:5188:PHE:HE2   | 4:d:5326:ARG:HG2   | 1.47                     | 0.79              |
| 5:e:5027:ILE:HB    | 5:e:5028:PRO:HD3   | 1.64                     | 0.79              |
| 15:u:5051:LYS:HG3  | 15:u:5052:ASN:H    | 1.48                     | 0.79              |
| 2:B:125:ASP:OD2    | 7:H:18:TYR:HB2     | 1.81                     | 0.79              |
| 2:B:464:PHE:CZ     | 28:B:1060:MGE:H4B1 | 2.18                     | 0.79              |
| 22:C:1029:CLA:CMA  | 22:C:1029:CLA:CBA  | 2.57                     | 0.79              |
| 1:a:5016:ARG:HA    | 1:a:5019:ASN:HD21  | 1.46                     | 0.79              |
| 23:a:6038:PHO:HBC3 | 23:a:6038:PHO:CHD  | 2.10                     | 0.79              |
| 2:b:5314:TYR:CE2   | 2:b:5316:GLY:HA3   | 2.17                     | 0.79              |
| 22:b:6011:CLA:O1A  | 22:b:6011:CLA:C4   | 2.30                     | 0.79              |
| 22:b:6012:CLA:CMD  | 22:b:6020:CLA:H201 | 2.13                     | 0.79              |
| 7:h:5043:LEU:HD21  | 17:x:5019:PHE:CZ   | 2.16                     | 0.79              |
| 3:C:307:PRO:HA     | 3:C:358:PHE:CD1    | 2.17                     | 0.79              |
| 22:C:1025:CLA:C15  | 22:C:1031:CLA:C9   | 2.49                     | 0.79              |
| 4:D:57:SER:CB      | 4:D:79:SER:HB3     | 2.13                     | 0.79              |
| 22:K:1034:CLA:H71  | 22:K:1034:CLA:H41  | 1.60                     | 0.79              |
| 1:a:5270:SER:HA    | 4:d:5232:PHE:CZ    | 2.17                     | 0.79              |
| 26:a:6063:LHG:H161 | 26:a:6063:LHG:C12  | 2.05                     | 0.79              |
| 22:b:6010:CLA:H12  | 22:b:6010:CLA:CBD  | 2.11                     | 0.79              |
| 22:b:6016:CLA:C16  | 22:d:6008:CLA:CMA  | 2.30                     | 0.79              |
| 3:c:5185:LEU:HG    | 3:c:5199:ILE:HD11  | 1.63                     | 0.79              |
| 2:B:468:TRP:HE1    | 22:B:1019:CLA:HED2 | 1.47                     | 0.79              |
| 3:C:167:VAL:O      | 22:C:1036:CLA:H41  | 1.83                     | 0.79              |
| 25:C:1054:BCR:H23C | 25:C:1054:BCR:H403 | 0.82                     | 0.79              |
| 16:V:70:GLY:HA3    | 16:V:156:TRP:O     | 1.83                     | 0.79              |
| 17:X:43:ILE:HG22   | 17:X:43:ILE:O      | 1.80                     | 0.79              |
| 3:c:5107:ASP:HB3   | 3:c:5110:PRO:HD2   | 1.65                     | 0.79              |
| 1:A:339:PHE:HB3    | 1:A:340:PRO:HD2    | 1.64                     | 0.79              |
| 23:A:1038:PHO:C9   | 22:D:1005:CLA:H18  | 2.11                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1009:CLA:CBD  | 22:B:1010:CLA:HBB1 | 1.94                     | 0.79              |
| 3:C:172:ALA:N      | 22:C:1025:CLA:CBC  | 2.46                     | 0.79              |
| 22:C:1026:CLA:O1A  | 22:C:1026:CLA:C2   | 2.30                     | 0.79              |
| 4:D:153:PHE:HB2    | 22:D:1004:CLA:H41  | 1.64                     | 0.79              |
| 4:D:317:LYS:NZ     | 27:D:1064:IOD:I    | 2.85                     | 0.79              |
| 23:D:1039:PHO:HMA3 | 22:D:1004:CLA:H143 | 1.57                     | 0.79              |
| 1:a:5224:ILE:HA    | 2:b:5482:ILE:HG12  | 1.64                     | 0.79              |
| 2:b:5332:LYS:HB3   | 2:b:5444:ARG:NH1   | 1.96                     | 0.79              |
| 22:b:6012:CLA:CMB  | 22:b:6015:CLA:HBB1 | 2.13                     | 0.79              |
| 22:b:6016:CLA:O1A  | 22:b:6016:CLA:CHA  | 2.30                     | 0.79              |
| 3:c:5050:LEU:HD21  | 3:c:5054:VAL:HG21  | 1.65                     | 0.79              |
| 3:c:5081:MET:HG3   | 3:c:5086:LEU:CD1   | 2.13                     | 0.79              |
| 3:c:5351:PHE:CE2   | 3:c:5375:LEU:HD11  | 2.18                     | 0.79              |
| 22:c:6029:CLA:CMA  | 22:c:6029:CLA:CBA  | 2.57                     | 0.79              |
| 10:k:5028:ILE:HD11 | 18:y:5028:ILE:HD12 | 1.65                     | 0.79              |
| 20:z:5046:LEU:O    | 20:z:5050:LEU:HB2  | 1.83                     | 0.79              |
| 1:A:116:ILE:HG23   | 1:A:117:PHE:H      | 1.47                     | 0.78              |
| 1:A:196:PRO:HG3    | 3:C:404:LEU:HD12   | 1.63                     | 0.78              |
| 1:A:215:HIS:NE2    | 1:A:271:LEU:HD11   | 1.97                     | 0.78              |
| 1:A:224:ILE:HA     | 2:B:482:ILE:CG1    | 2.13                     | 0.78              |
| 2:B:99:ALA:HB1     | 22:B:1014:CLA:H42  | 1.64                     | 0.78              |
| 22:B:1012:CLA:C1D  | 22:B:1020:CLA:H202 | 2.12                     | 0.78              |
| 22:B:1012:CLA:CMD  | 22:B:1020:CLA:H201 | 2.13                     | 0.78              |
| 22:B:1013:CLA:C3B  | 22:B:1014:CLA:H51  | 2.13                     | 0.78              |
| 3:C:107:ASP:HB3    | 3:C:110:PRO:HD2    | 1.65                     | 0.78              |
| 1:a:5224:ILE:HA    | 2:b:5482:ILE:CG1   | 2.13                     | 0.78              |
| 2:b:5080:ILE:HD11  | 2:b:5093:PHE:HZ    | 1.45                     | 0.78              |
| 22:b:6009:CLA:C1A  | 22:b:6009:CLA:O1A  | 2.30                     | 0.78              |
| 22:b:6013:CLA:C3B  | 22:b:6014:CLA:H51  | 2.13                     | 0.78              |
| 3:c:5167:VAL:O     | 22:c:6036:CLA:H41  | 1.83                     | 0.78              |
| 4:d:5146:PHE:O     | 4:d:5149:PRO:HD2   | 1.82                     | 0.78              |
| 15:u:5028:ASN:HD22 | 15:u:5054:PRO:HB2  | 1.46                     | 0.78              |
| 16:v:5092:ARG:HH11 | 16:v:5092:ARG:HG3  | 1.48                     | 0.78              |
| 25:B:1047:BCR:H341 | 25:B:1047:BCR:C12  | 2.12                     | 0.78              |
| 3:C:220:GLY:O      | 3:C:221:GLU:HG3    | 1.81                     | 0.78              |
| 22:C:1025:CLA:H151 | 22:C:1031:CLA:H91  | 1.64                     | 0.78              |
| 22:C:1028:CLA:H91  | 29:C:1056:DGD:HBT1 | 1.65                     | 0.78              |
| 22:C:1031:CLA:OBD  | 22:C:1033:CLA:C12  | 2.28                     | 0.78              |
| 6:F:45:ARG:HA      | 6:F:45:ARG:NE      | 1.97                     | 0.78              |
| 3:c:5171:GLY:CA    | 3:c:5174:LEU:HB2   | 2.11                     | 0.78              |
| 3:c:5428:THR:HG23  | 3:c:5429:SER:H     | 1.46                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:k:6034:CLA:H143 | 22:k:6034:CLA:C10  | 2.06                     | 0.78              |
| 22:B:1012:CLA:C2B  | 22:B:1015:CLA:CBB  | 2.62                     | 0.78              |
| 3:C:397:THR:OG1    | 3:C:398:HIS:ND1    | 2.17                     | 0.78              |
| 28:L:1061:MGE:O1B  | 28:L:1061:MGE:C1G  | 2.31                     | 0.78              |
| 1:a:5091:LEU:HG    | 1:a:5166:GLY:O     | 1.83                     | 0.78              |
| 23:a:6038:PHO:H201 | 22:d:6005:CLA:CMB  | 2.13                     | 0.78              |
| 22:b:6012:CLA:C2B  | 22:b:6015:CLA:HBB2 | 2.14                     | 0.78              |
| 22:c:6025:CLA:HMB2 | 25:c:6054:BCR:C25  | 2.14                     | 0.78              |
| 22:c:6036:CLA:HMC3 | 22:c:6036:CLA:HBC2 | 1.65                     | 0.78              |
| 4:d:5317:LYS:NZ    | 27:d:6064:IOD:I    | 2.85                     | 0.78              |
| 7:h:5038:PHE:HB2   | 25:h:6049:BCR:H10C | 1.64                     | 0.78              |
| 2:B:105:GLY:HA2    | 25:B:1047:BCR:H402 | 1.64                     | 0.78              |
| 2:B:108:PHE:O      | 2:B:111:ALA:HB3    | 1.83                     | 0.78              |
| 22:B:1022:CLA:HHD  | 22:B:1022:CLA:CBC  | 2.09                     | 0.78              |
| 1:a:5172:MET:HE3   | 1:a:5182:PHE:HD2   | 1.49                     | 0.78              |
| 3:c:5420:VAL:HB    | 3:c:5425:TRP:HE1   | 1.49                     | 0.78              |
| 18:y:5043:ARG:CD   | 18:y:5044:GLY:H    | 1.95                     | 0.78              |
| 22:B:1012:CLA:C2B  | 22:B:1015:CLA:HBB2 | 2.14                     | 0.78              |
| 22:C:1029:CLA:H42  | 22:C:1029:CLA:CHD  | 2.13                     | 0.78              |
| 4:D:328:TRP:HZ3    | 16:V:161:VAL:HA    | 1.49                     | 0.78              |
| 22:a:6007:CLA:HBA2 | 22:a:6007:CLA:HBD  | 1.64                     | 0.78              |
| 2:b:5174:LEU:CD2   | 2:b:5312:TYR:OH    | 2.31                     | 0.78              |
| 2:b:5464:PHE:CZ    | 28:b:6060:MGE:H4B1 | 2.18                     | 0.78              |
| 3:c:5172:ALA:N     | 22:c:6025:CLA:CBC  | 2.46                     | 0.78              |
| 22:c:6029:CLA:H43  | 25:c:6054:BCR:H321 | 1.63                     | 0.78              |
| 1:A:143:ILE:HB     | 4:D:220:ASN:ND2    | 1.99                     | 0.78              |
| 22:A:1007:CLA:H43  | 22:C:1029:CLA:C19  | 2.14                     | 0.78              |
| 2:B:49:ASP:CB      | 13:o:5083:LYS:HE3  | 2.14                     | 0.78              |
| 22:B:1023:CLA:C9   | 22:B:1024:CLA:H151 | 2.13                     | 0.78              |
| 6:F:19:ARG:O       | 6:F:23:VAL:HG23    | 1.84                     | 0.78              |
| 11:L:21:LEU:HB2    | 14:T:16:LEU:HD21   | 1.64                     | 0.78              |
| 1:a:5196:PRO:HG3   | 3:c:5404:LEU:HD12  | 1.63                     | 0.78              |
| 1:a:5278:TRP:HA    | 1:a:5278:TRP:HE3   | 1.46                     | 0.78              |
| 22:b:6012:CLA:C2B  | 22:b:6015:CLA:CBB  | 2.62                     | 0.78              |
| 22:B:1010:CLA:H151 | 29:B:1058:DGD:HA82 | 1.64                     | 0.78              |
| 3:C:420:VAL:HB     | 3:C:425:TRP:HE1    | 1.49                     | 0.78              |
| 22:C:1025:CLA:HMB2 | 25:C:1054:BCR:C25  | 2.13                     | 0.78              |
| 22:C:1029:CLA:HMC1 | 22:C:1029:CLA:HBC3 | 1.66                     | 0.78              |
| 10:K:28:ILE:HD11   | 18:Y:28:ILE:HD12   | 1.65                     | 0.78              |
| 13:O:243:SER:OG    | 13:O:261:ILE:HB    | 1.82                     | 0.78              |
| 22:b:6009:CLA:CAA  | 22:b:6009:CLA:O2D  | 2.30                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6021:CLA:H142 | 22:b:6021:CLA:H101 | 1.65                     | 0.78              |
| 22:c:6029:CLA:H42  | 22:c:6029:CLA:CHD  | 2.13                     | 0.78              |
| 22:c:6033:CLA:H141 | 22:c:6036:CLA:C2D  | 2.14                     | 0.78              |
| 5:e:5034:GLY:HA2   | 6:f:5032:PHE:CE1   | 2.19                     | 0.78              |
| 13:o:5052:ALA:HB1  | 13:o:5230:VAL:N    | 1.99                     | 0.78              |
| 16:v:5070:GLY:HA3  | 16:v:5156:TRP:O    | 1.83                     | 0.78              |
| 3:C:56:HIS:C       | 3:C:56:HIS:CD2     | 2.62                     | 0.78              |
| 3:C:121:SER:O      | 3:C:124:VAL:HG22   | 1.84                     | 0.78              |
| 5:E:27:ILE:HB      | 5:E:28:PRO:HD3     | 1.64                     | 0.78              |
| 22:c:6030:CLA:H172 | 22:c:6030:CLA:H122 | 1.62                     | 0.78              |
| 10:k:5031:LEU:HB3  | 25:k:6051:BCR:H14C | 1.63                     | 0.78              |
| 22:B:1022:CLA:H11  | 22:B:1022:CLA:C3D  | 2.14                     | 0.78              |
| 22:C:1030:CLA:C3D  | 22:C:1030:CLA:CED  | 2.62                     | 0.78              |
| 18:Y:42:ARG:O      | 18:Y:43:ARG:HB3    | 1.83                     | 0.78              |
| 25:b:6047:BCR:H371 | 25:b:6047:BCR:H403 | 1.33                     | 0.78              |
| 3:c:5292:PHE:CD1   | 29:c:6055:DGD:HD1  | 2.18                     | 0.78              |
| 1:A:91:LEU:HG      | 1:A:166:GLY:O      | 1.83                     | 0.78              |
| 22:B:1012:CLA:CMB  | 22:B:1015:CLA:HBB1 | 2.12                     | 0.78              |
| 3:C:42:LEU:HD11    | 3:C:49:LEU:HD12    | 1.66                     | 0.78              |
| 3:C:92:ILE:HD12    | 3:C:92:ILE:N       | 1.99                     | 0.78              |
| 22:C:1030:CLA:HBC2 | 22:C:1030:CLA:CHD  | 2.13                     | 0.78              |
| 22:C:1037:CLA:HBC2 | 22:C:1037:CLA:CHD  | 2.12                     | 0.78              |
| 22:K:1034:CLA:CGA  | 22:K:1034:CLA:H42  | 2.14                     | 0.78              |
| 20:z:5055:GLY:HA2  | 25:z:6053:BCR:H311 | 1.65                     | 0.78              |
| 2:B:260:SER:OG     | 2:B:262:THR:HG23   | 1.83                     | 0.77              |
| 3:C:171:GLY:CA     | 3:C:174:LEU:HB2    | 2.11                     | 0.77              |
| 22:D:1004:CLA:H102 | 22:D:1004:CLA:H142 | 1.66                     | 0.77              |
| 10:K:37:PHE:HB3    | 25:K:1051:BCR:H401 | 1.66                     | 0.77              |
| 20:Z:46:LEU:O      | 20:Z:50:LEU:HB2    | 1.83                     | 0.77              |
| 22:b:6021:CLA:OBD  | 22:b:6022:CLA:CHC  | 2.32                     | 0.77              |
| 3:c:5092:ILE:HD12  | 3:c:5092:ILE:N     | 1.99                     | 0.77              |
| 3:c:5397:THR:OG1   | 3:c:5398:HIS:ND1   | 2.17                     | 0.77              |
| 13:o:5141:ARG:HG2  | 13:o:5141:ARG:NH1  | 1.96                     | 0.77              |
| 22:C:1025:CLA:H43  | 22:C:1025:CLA:C1B  | 2.14                     | 0.77              |
| 10:K:18:PHE:O      | 10:K:22:VAL:HG23   | 1.85                     | 0.77              |
| 16:V:64:ALA:O      | 16:V:68:VAL:CG1    | 2.26                     | 0.77              |
| 1:a:5215:HIS:NE2   | 1:a:5271:LEU:HD11  | 1.97                     | 0.77              |
| 22:b:6011:CLA:O1A  | 22:b:6011:CLA:H43  | 1.85                     | 0.77              |
| 22:b:6022:CLA:C14  | 22:b:6022:CLA:C8   | 2.61                     | 0.77              |
| 22:b:6022:CLA:HBC3 | 22:b:6022:CLA:H91  | 1.66                     | 0.77              |
| 3:c:5056:HIS:C     | 3:c:5056:HIS:CD2   | 2.62                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5297:ASP:CG    | 4:d:5298:PHE:H     | 1.89                     | 0.77              |
| 17:x:5025:SER:O    | 17:x:5029:VAL:HG23 | 1.84                     | 0.77              |
| 22:A:1003:CLA:CAA  | 22:A:1003:CLA:CED  | 2.30                     | 0.77              |
| 22:B:1021:CLA:OBD  | 22:B:1022:CLA:CHC  | 2.32                     | 0.77              |
| 3:C:343:ARG:HH12   | 3:C:348:GLU:HG3    | 0.74                     | 0.77              |
| 22:C:1030:CLA:HED3 | 22:C:1030:CLA:C4D  | 2.15                     | 0.77              |
| 4:D:148:ALA:O      | 4:D:152:VAL:HG23   | 1.84                     | 0.77              |
| 4:D:246:MET:HE3    | 4:D:264:LYS:CG     | 2.14                     | 0.77              |
| 5:E:34:GLY:HA2     | 6:F:32:PHE:CE1     | 2.19                     | 0.77              |
| 13:O:82:PRO:CG     | 13:O:89:ALA:HB1    | 2.15                     | 0.77              |
| 13:O:172:PHE:HB2   | 13:O:221:GLY:H     | 1.49                     | 0.77              |
| 15:U:51:LYS:HG3    | 15:U:52:ASN:H      | 1.48                     | 0.77              |
| 17:X:25:SER:O      | 17:X:29:VAL:HG23   | 1.84                     | 0.77              |
| 3:c:5171:GLY:C     | 22:c:6025:CLA:CBC  | 2.58                     | 0.77              |
| 3:c:5202:PRO:HB3   | 3:c:5235:GLY:HA2   | 1.67                     | 0.77              |
| 22:c:6025:CLA:O2A  | 22:c:6025:CLA:C4A  | 2.32                     | 0.77              |
| 4:d:5201:VAL:CG2   | 22:d:6004:CLA:HMB2 | 2.12                     | 0.77              |
| 6:f:5019:ARG:O     | 6:f:5023:VAL:HG23  | 1.84                     | 0.77              |
| 14:t:5014:ILE:O    | 14:t:5017:PHE:HB2  | 1.85                     | 0.77              |
| 22:A:1007:CLA:HBA2 | 22:A:1007:CLA:HBD  | 1.64                     | 0.77              |
| 2:B:249:ALA:HB2    | 22:B:1012:CLA:CBC  | 2.15                     | 0.77              |
| 3:C:49:LEU:CD1     | 22:C:1035:CLA:HMA2 | 2.14                     | 0.77              |
| 29:C:1057:DGD:HBG2 | 29:C:1057:DGD:CEB  | 2.10                     | 0.77              |
| 10:K:21:LEU:HD11   | 18:Y:24:MET:HG3    | 1.66                     | 0.77              |
| 2:b:5249:ALA:HB2   | 22:b:6012:CLA:CBC  | 2.15                     | 0.77              |
| 3:c:5164:HIS:O     | 3:c:5168:LEU:HD13  | 1.85                     | 0.77              |
| 22:k:6034:CLA:H71  | 22:k:6034:CLA:H41  | 1.60                     | 0.77              |
| 22:k:6034:CLA:CGA  | 22:k:6034:CLA:H42  | 2.14                     | 0.77              |
| 1:A:172:MET:HE3    | 1:A:182:PHE:HD2    | 1.49                     | 0.77              |
| 22:A:1007:CLA:HED2 | 22:A:1007:CLA:CAD  | 2.15                     | 0.77              |
| 3:C:49:LEU:HD21    | 22:C:1035:CLA:CMA  | 2.15                     | 0.77              |
| 1:a:5116:ILE:HG23  | 1:a:5117:PHE:H     | 1.47                     | 0.77              |
| 2:b:5108:PHE:O     | 2:b:5111:ALA:HB3   | 1.84                     | 0.77              |
| 22:c:6026:CLA:O1A  | 22:c:6026:CLA:C2   | 2.30                     | 0.77              |
| 22:c:6031:CLA:O2A  | 22:c:6031:CLA:CMA  | 2.32                     | 0.77              |
| 13:o:5172:PHE:HB2  | 13:o:5221:GLY:H    | 1.49                     | 0.77              |
| 20:z:5015:LEU:HD12 | 20:z:5050:LEU:HD12 | 1.66                     | 0.77              |
| 4:D:36:LEU:HD21    | 4:D:124:GLY:HA2    | 1.66                     | 0.77              |
| 13:O:52:ALA:HB1    | 13:O:230:VAL:N     | 1.99                     | 0.77              |
| 16:V:125:ASP:HA    | 16:V:131:ARG:HH21  | 1.50                     | 0.77              |
| 22:a:6007:CLA:H43  | 22:c:6029:CLA:C19  | 2.14                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5260:SER:OG    | 2:b:5262:THR:HG23  | 1.83                     | 0.77              |
| 22:b:6023:CLA:C13  | 22:b:6024:CLA:HMA3 | 2.09                     | 0.77              |
| 22:c:6026:CLA:O1A  | 22:c:6026:CLA:C3   | 2.33                     | 0.77              |
| 29:c:6055:DGD:HA72 | 29:c:6055:DGD:HAW2 | 1.65                     | 0.77              |
| 4:d:5191:TRP:CZ2   | 4:d:5197:HIS:HB2   | 2.20                     | 0.77              |
| 24:A:1043:PQ9:C45  | 28:D:1059:MGE:CAA  | 2.57                     | 0.77              |
| 22:C:1025:CLA:O2A  | 22:C:1025:CLA:C4A  | 2.32                     | 0.77              |
| 1:a:5094:TYR:HE1   | 1:a:5105:TRP:HA    | 1.49                     | 0.77              |
| 4:d:5055:VAL:HG21  | 4:d:5110:LEU:HD21  | 1.67                     | 0.77              |
| 13:o:5031:LEU:HD13 | 13:o:5036:ILE:HD11 | 1.64                     | 0.77              |
| 18:y:5042:ARG:O    | 18:y:5043:ARG:HB3  | 1.83                     | 0.77              |
| 22:A:1006:CLA:H161 | 25:D:1050:BCR:H272 | 1.64                     | 0.77              |
| 22:C:1029:CLA:HHC  | 22:C:1029:CLA:HBB1 | 1.65                     | 0.77              |
| 4:D:184:PHE:HE2    | 4:D:188:PHE:CD1    | 2.03                     | 0.77              |
| 22:b:6009:CLA:HBA1 | 22:b:6009:CLA:CBD  | 2.15                     | 0.77              |
| 22:b:6011:CLA:C3D  | 22:b:6013:CLA:C1   | 2.63                     | 0.77              |
| 3:c:5121:SER:O     | 3:c:5124:VAL:HG22  | 1.84                     | 0.77              |
| 3:c:5403:SER:OG    | 3:c:5407:VAL:HG12  | 1.85                     | 0.77              |
| 22:c:6029:CLA:HHC  | 22:c:6029:CLA:HBB1 | 1.65                     | 0.77              |
| 22:c:6030:CLA:C4D  | 22:c:6030:CLA:HED3 | 2.15                     | 0.77              |
| 4:d:5148:ALA:O     | 4:d:5152:VAL:HG23  | 1.84                     | 0.77              |
| 22:d:6004:CLA:H102 | 22:d:6004:CLA:H142 | 1.67                     | 0.77              |
| 22:B:1024:CLA:H2A  | 22:B:1024:CLA:O2A  | 1.83                     | 0.77              |
| 3:C:81:MET:HG3     | 3:C:86:LEU:CD1     | 2.13                     | 0.77              |
| 25:D:1050:BCR:C20  | 28:D:1059:MGE:H5A1 | 2.15                     | 0.77              |
| 22:b:6022:CLA:H11  | 22:b:6022:CLA:C3D  | 2.14                     | 0.77              |
| 4:d:5089:LEU:HD12  | 7:h:5050:ASN:OD1   | 1.85                     | 0.77              |
| 23:d:6039:PHO:HBC2 | 23:d:6039:PHO:HHD  | 1.67                     | 0.77              |
| 10:k:5021:LEU:HD11 | 18:y:5024:MET:HG3  | 1.66                     | 0.77              |
| 2:B:5:TRP:O        | 2:B:8:VAL:HG13     | 1.85                     | 0.77              |
| 22:B:1009:CLA:HAA1 | 25:H:1049:BCR:H363 | 1.66                     | 0.77              |
| 22:B:1012:CLA:CGA  | 22:B:1020:CLA:C14  | 2.63                     | 0.77              |
| 22:B:1021:CLA:H142 | 22:B:1021:CLA:H101 | 1.65                     | 0.77              |
| 3:C:171:GLY:C      | 22:C:1025:CLA:CBC  | 2.58                     | 0.77              |
| 3:C:199:ILE:HG21   | 3:C:234:VAL:CG1    | 2.15                     | 0.77              |
| 22:C:1035:CLA:C9   | 25:C:1052:BCR:C40  | 2.63                     | 0.77              |
| 4:D:188:PHE:HE2    | 4:D:326:ARG:HG2    | 1.47                     | 0.77              |
| 28:b:6060:MGE:H212 | 28:b:6060:MGE:H251 | 0.79                     | 0.77              |
| 22:c:6029:CLA:HMC1 | 22:c:6029:CLA:HBC3 | 1.66                     | 0.77              |
| 4:d:5261:PHE:CE2   | 4:d:5267:LEU:HA    | 2.20                     | 0.77              |
| 22:B:1009:CLA:H3A  | 25:H:1049:BCR:H372 | 1.67                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1011:CLA:O1A  | 22:B:1011:CLA:C3A  | 2.30                     | 0.76              |
| 3:C:224:ILE:HG23   | 25:C:1054:BCR:C38  | 2.15                     | 0.76              |
| 3:C:351:PHE:CE2    | 3:C:375:LEU:HD11   | 2.18                     | 0.76              |
| 29:C:1055:DGD:HA72 | 29:C:1055:DGD:HAW2 | 1.65                     | 0.76              |
| 18:Y:25:ILE:HG13   | 18:Y:26:ALA:N      | 2.00                     | 0.76              |
| 2:b:5249:ALA:O     | 2:b:5252:VAL:HG12  | 1.85                     | 0.76              |
| 22:b:6022:CLA:O1D  | 22:b:6022:CLA:CAA  | 2.30                     | 0.76              |
| 22:c:6025:CLA:H43  | 22:c:6025:CLA:C1B  | 2.14                     | 0.76              |
| 2:B:249:ALA:O      | 2:B:252:VAL:HG12   | 1.85                     | 0.76              |
| 22:B:1009:CLA:HMB3 | 25:H:1049:BCR:C27  | 1.98                     | 0.76              |
| 22:C:1037:CLA:O2D  | 22:C:1037:CLA:H2A  | 1.85                     | 0.76              |
| 4:D:89:LEU:HD12    | 7:H:50:ASN:OD1     | 1.85                     | 0.76              |
| 4:D:191:TRP:CZ2    | 4:D:197:HIS:HB2    | 2.20                     | 0.76              |
| 4:D:261:PHE:CE2    | 4:D:267:LEU:HA     | 2.20                     | 0.76              |
| 1:a:5143:ILE:HB    | 4:d:5220:ASN:ND2   | 1.99                     | 0.76              |
| 2:b:5246:PHE:O     | 2:b:5249:ALA:HB3   | 1.85                     | 0.76              |
| 2:b:5460:LEU:HA    | 29:b:6058:DGD:CIA  | 2.15                     | 0.76              |
| 22:b:6011:CLA:C1   | 22:b:6013:CLA:C9   | 2.63                     | 0.76              |
| 3:c:5472:LEU:O     | 3:c:5473:ASP:HB2   | 1.85                     | 0.76              |
| 22:c:6030:CLA:HBC2 | 22:c:6030:CLA:CHD  | 2.13                     | 0.76              |
| 22:c:6030:CLA:C3D  | 22:c:6030:CLA:CED  | 2.62                     | 0.76              |
| 22:c:6033:CLA:CMA  | 22:k:6034:CLA:HAC1 | 2.16                     | 0.76              |
| 13:o:5082:PRO:HG3  | 13:o:5089:ALA:HB1  | 1.68                     | 0.76              |
| 1:A:197:PHE:HE1    | 1:A:285:PHE:HD2    | 1.33                     | 0.76              |
| 22:A:1003:CLA:H71  | 22:A:1003:CLA:H43  | 1.67                     | 0.76              |
| 23:A:1038:PHO:H201 | 22:D:1005:CLA:CMB  | 2.13                     | 0.76              |
| 2:B:112:CYS:SG     | 14:t:5023:PHE:HZ   | 2.08                     | 0.76              |
| 2:B:392:PHE:HA     | 2:B:397:VAL:HG23   | 1.68                     | 0.76              |
| 22:C:1036:CLA:HMC3 | 22:C:1036:CLA:HBC2 | 1.65                     | 0.76              |
| 22:a:6006:CLA:HBC3 | 22:a:6006:CLA:CHD  | 2.11                     | 0.76              |
| 22:b:6022:CLA:C1A  | 22:b:6022:CLA:O2A  | 2.34                     | 0.76              |
| 22:c:6037:CLA:O2D  | 22:c:6037:CLA:H2A  | 1.85                     | 0.76              |
| 13:o:5223:ILE:CG2  | 13:o:5243:SER:HB3  | 2.15                     | 0.76              |
| 16:v:5064:ALA:O    | 16:v:5068:VAL:CG1  | 2.26                     | 0.76              |
| 1:A:246:TYR:HD1    | 1:A:246:TYR:H      | 1.34                     | 0.76              |
| 22:B:1011:CLA:C1   | 22:B:1013:CLA:C9   | 2.63                     | 0.76              |
| 22:B:1016:CLA:H52  | 22:H:1017:CLA:H112 | 1.63                     | 0.76              |
| 3:C:164:HIS:O      | 3:C:168:LEU:HD13   | 1.85                     | 0.76              |
| 22:C:1033:CLA:H141 | 22:C:1036:CLA:C2D  | 2.14                     | 0.76              |
| 22:a:6006:CLA:HBC1 | 4:d:5182:LEU:HD21  | 1.68                     | 0.76              |
| 7:h:5017:GLU:HB2   | 7:h:5020:LYS:HB2   | 1.67                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1009:CLA:H121 | 22:B:1009:CLA:H91  | 0.83                     | 0.76              |
| 3:C:403:SER:OG     | 3:C:407:VAL:HG12   | 1.85                     | 0.76              |
| 22:C:1031:CLA:O2A  | 22:C:1031:CLA:CMA  | 2.32                     | 0.76              |
| 4:D:55:VAL:HG21    | 4:D:110:LEU:HD21   | 1.67                     | 0.76              |
| 4:D:201:VAL:CG2    | 22:D:1004:CLA:HMB2 | 2.12                     | 0.76              |
| 25:T:6048:BCR:H331 | 25:T:6048:BCR:C8   | 2.15                     | 0.76              |
| 16:V:98:LEU:H      | 16:V:98:LEU:CD2    | 1.97                     | 0.76              |
| 22:c:6033:CLA:CED  | 22:c:6033:CLA:CAD  | 2.64                     | 0.76              |
| 25:d:6050:BCR:C20  | 28:d:6059:MGE:H5A1 | 2.15                     | 0.76              |
| 26:A:1063:LHG:C32  | 22:K:1034:CLA:H151 | 2.16                     | 0.76              |
| 22:B:1009:CLA:C8   | 22:B:1009:CLA:H142 | 2.09                     | 0.76              |
| 22:B:1011:CLA:O1A  | 22:B:1011:CLA:H43  | 1.85                     | 0.76              |
| 22:B:1023:CLA:C13  | 22:B:1024:CLA:HMA3 | 2.09                     | 0.76              |
| 16:V:92:ARG:HG3    | 16:V:92:ARG:HH11   | 1.48                     | 0.76              |
| 20:Z:15:LEU:HD12   | 20:Z:50:LEU:HD12   | 1.66                     | 0.76              |
| 1:a:5197:PHE:HE1   | 1:a:5285:PHE:HD2   | 1.33                     | 0.76              |
| 22:b:6021:CLA:CED  | 22:b:6021:CLA:O1A  | 2.34                     | 0.76              |
| 22:c:6037:CLA:HBC2 | 22:c:6037:CLA:CHD  | 2.12                     | 0.76              |
| 10:k:5018:PHE:O    | 10:k:5022:VAL:HG23 | 1.85                     | 0.76              |
| 16:v:5125:ASP:HA   | 16:v:5131:ARG:HH21 | 1.50                     | 0.76              |
| 22:B:1011:CLA:C3D  | 22:B:1013:CLA:C1   | 2.63                     | 0.76              |
| 22:B:1019:CLA:HBB1 | 22:B:1019:CLA:HHC  | 1.67                     | 0.76              |
| 22:C:1026:CLA:O1A  | 22:C:1026:CLA:C3   | 2.33                     | 0.76              |
| 22:C:1031:CLA:C14  | 25:C:1054:BCR:C36  | 2.64                     | 0.76              |
| 4:D:297:ASP:CG     | 4:D:298:PHE:H      | 1.89                     | 0.76              |
| 13:O:223:ILE:CG2   | 13:O:243:SER:HB3   | 2.15                     | 0.76              |
| 22:a:6006:CLA:C17  | 25:d:6050:BCR:H272 | 2.16                     | 0.76              |
| 26:a:6063:LHG:C32  | 22:k:6034:CLA:H151 | 2.16                     | 0.76              |
| 22:b:6012:CLA:CGA  | 22:b:6020:CLA:C14  | 2.63                     | 0.76              |
| 3:c:5224:ILE:HG23  | 25:c:6054:BCR:C38  | 2.15                     | 0.76              |
| 22:c:6025:CLA:C15  | 22:c:6031:CLA:C9   | 2.49                     | 0.76              |
| 4:d:5169:PHE:C     | 27:d:6068:IOD:I    | 2.98                     | 0.76              |
| 4:d:5328:TRP:HZ3   | 16:v:5161:VAL:HA   | 1.49                     | 0.76              |
| 15:u:5043:PRO:HG3  | 16:v:5109:ASP:N    | 2.01                     | 0.76              |
| 16:v:5098:LEU:H    | 16:v:5098:LEU:CD2  | 1.97                     | 0.76              |
| 1:A:29:TYR:CD2     | 1:A:133:LEU:HD13   | 2.21                     | 0.76              |
| 2:B:460:LEU:HA     | 29:B:1058:DGD:CIA  | 2.15                     | 0.76              |
| 25:B:1048:BCR:H331 | 25:B:1048:BCR:C8   | 2.15                     | 0.76              |
| 3:C:202:PRO:HB3    | 3:C:235:GLY:HA2    | 1.67                     | 0.76              |
| 29:C:1056:DGD:O1A  | 29:C:1056:DGD:C4A  | 2.34                     | 0.76              |
| 16:V:151:ILE:H     | 16:V:151:ILE:HD13  | 1.51                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6030:CLA:HBB1 | 22:c:6030:CLA:CHC  | 2.15                     | 0.76              |
| 22:c:6035:CLA:C9   | 25:k:6052:BCR:C40  | 2.63                     | 0.76              |
| 2:B:174:LEU:CD2    | 2:B:312:TYR:OH     | 2.31                     | 0.76              |
| 22:B:1009:CLA:H8   | 22:B:1009:CLA:H142 | 1.62                     | 0.76              |
| 22:B:1009:CLA:CAA  | 22:B:1009:CLA:O2D  | 2.30                     | 0.76              |
| 22:B:1022:CLA:H93  | 22:B:1022:CLA:H122 | 1.63                     | 0.76              |
| 3:c:5199:ILE:HG21  | 3:c:5234:VAL:CG1   | 2.15                     | 0.76              |
| 22:B:1022:CLA:C14  | 22:B:1022:CLA:C8   | 2.61                     | 0.76              |
| 22:B:1022:CLA:HBC3 | 22:B:1022:CLA:H91  | 1.66                     | 0.76              |
| 22:B:1022:CLA:O2A  | 22:B:1022:CLA:C1A  | 2.34                     | 0.76              |
| 3:C:56:HIS:HD2     | 3:C:57:ALA:N       | 1.84                     | 0.76              |
| 3:C:167:VAL:HG11   | 22:C:1036:CLA:HBA2 | 1.67                     | 0.76              |
| 22:C:1033:CLA:CED  | 22:C:1033:CLA:CAD  | 2.64                     | 0.76              |
| 4:D:139:ARG:NH1    | 4:D:265:ARG:NH2    | 2.28                     | 0.76              |
| 7:H:7:LEU:HD23     | 7:H:10:ILE:HD12    | 1.68                     | 0.76              |
| 15:U:43:PRO:HG3    | 16:V:109:ASP:N     | 2.01                     | 0.76              |
| 3:c:5075:PHE:HZ    | 3:c:5105:VAL:HG11  | 1.51                     | 0.76              |
| 3:C:75:PHE:HZ      | 3:C:105:VAL:HG11   | 1.51                     | 0.75              |
| 3:C:109:PHE:HB3    | 3:C:110:PRO:HD3    | 1.67                     | 0.75              |
| 3:C:249:ILE:O      | 3:C:252:ILE:HG22   | 1.86                     | 0.75              |
| 4:D:226:GLY:HA3    | 4:D:234:ALA:CB     | 2.16                     | 0.75              |
| 14:T:14:ILE:O      | 14:T:17:PHE:HB2    | 1.85                     | 0.75              |
| 1:a:5029:TYR:CD2   | 1:a:5133:LEU:HD13  | 2.21                     | 0.75              |
| 1:a:5126:TYR:HD2   | 1:a:5126:TYR:O     | 1.69                     | 0.75              |
| 1:a:5219:VAL:HG21  | 4:d:5268:HIS:CD2   | 2.21                     | 0.75              |
| 2:b:5298:LEU:HD11  | 2:b:5302:TRP:HE1   | 1.51                     | 0.75              |
| 22:c:6031:CLA:C14  | 25:c:6054:BCR:C36  | 2.64                     | 0.75              |
| 4:d:5118:GLY:CA    | 23:d:6039:PHO:H8   | 2.16                     | 0.75              |
| 10:k:5035:LEU:HA   | 10:k:5038:VAL:CG2  | 2.16                     | 0.75              |
| 28:l:6061:MGE:O1B  | 28:l:6061:MGE:C1G  | 2.31                     | 0.75              |
| 18:y:5025:ILE:HG13 | 18:y:5026:ALA:N    | 2.00                     | 0.75              |
| 22:A:1006:CLA:HBC3 | 22:A:1006:CLA:CHD  | 2.11                     | 0.75              |
| 2:B:246:PHE:O      | 2:B:249:ALA:HB3    | 1.85                     | 0.75              |
| 2:B:298:LEU:HD11   | 2:B:302:TRP:HE1    | 1.51                     | 0.75              |
| 22:B:1022:CLA:O1D  | 22:B:1022:CLA:CAA  | 2.30                     | 0.75              |
| 4:D:240:ALA:O      | 4:D:241:GLU:HG3    | 1.87                     | 0.75              |
| 23:D:1039:PHO:HBC2 | 23:D:1039:PHO:HHH  | 1.67                     | 0.75              |
| 5:E:13:ILE:HA      | 5:E:16:SER:CB      | 2.16                     | 0.75              |
| 1:a:5272:HIS:CB    | 4:d:5218:VAL:HG11  | 2.17                     | 0.75              |
| 22:b:6014:CLA:HBC2 | 22:b:6014:CLA:CHD  | 2.11                     | 0.75              |
| 22:b:6016:CLA:C5   | 22:h:6017:CLA:C9   | 2.34                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5167:VAL:HG11  | 22:c:6036:CLA:HBA2 | 1.67                     | 0.75              |
| 22:c:6031:CLA:HAA1 | 22:c:6033:CLA:HED2 | 1.68                     | 0.75              |
| 13:o:5082:PRO:CG   | 13:o:5089:ALA:HB1  | 2.15                     | 0.75              |
| 1:A:94:TYR:HE1     | 1:A:105:TRP:HA     | 1.49                     | 0.75              |
| 22:A:1006:CLA:C17  | 25:D:1050:BCR:H272 | 2.16                     | 0.75              |
| 2:B:52:LEU:HD22    | 2:B:311:PHE:CD1    | 2.21                     | 0.75              |
| 4:D:51:GLY:HA2     | 4:D:55:VAL:HB      | 1.69                     | 0.75              |
| 2:b:5052:LEU:HD22  | 2:b:5311:PHE:CD1   | 2.21                     | 0.75              |
| 3:c:5117:VAL:HG11  | 22:c:6027:CLA:C4   | 2.15                     | 0.75              |
| 22:c:6033:CLA:HMA3 | 22:k:6034:CLA:CMC  | 2.16                     | 0.75              |
| 4:d:5240:ALA:O     | 4:d:5241:GLU:HG3   | 1.87                     | 0.75              |
| 7:h:5007:LEU:HD23  | 7:h:5010:ILE:HD12  | 1.68                     | 0.75              |
| 1:A:224:ILE:N      | 2:B:482:ILE:HG23   | 2.01                     | 0.75              |
| 3:C:117:VAL:HG11   | 22:C:1027:CLA:C4   | 2.15                     | 0.75              |
| 2:b:5005:TRP:O     | 2:b:5008:VAL:HG13  | 1.85                     | 0.75              |
| 22:b:6013:CLA:CMB  | 22:b:6014:CLA:H11  | 2.16                     | 0.75              |
| 22:c:6030:CLA:HBB2 | 22:c:6031:CLA:CED  | 2.16                     | 0.75              |
| 29:c:6056:DGD:O1A  | 29:c:6056:DGD:C4A  | 2.34                     | 0.75              |
| 4:d:5036:LEU:HD21  | 4:d:5124:GLY:HA2   | 1.66                     | 0.75              |
| 4:d:5051:GLY:HA2   | 4:d:5055:VAL:HB    | 1.69                     | 0.75              |
| 4:d:5226:GLY:HA3   | 4:d:5234:ALA:CB    | 2.16                     | 0.75              |
| 13:o:5080:GLU:O    | 13:o:5082:PRO:CD   | 2.33                     | 0.75              |
| 14:t:5018:PHE:HD1  | 25:t:1046:BCR:H332 | 1.49                     | 0.75              |
| 1:a:5293:MET:HG2   | 1:a:5298:ASN:HA    | 1.68                     | 0.75              |
| 2:b:5191:ASN:ND2   | 7:h:5060:VAL:HA    | 2.02                     | 0.75              |
| 2:b:5384:ARG:HD3   | 15:u:5102:LEU:HD21 | 1.69                     | 0.75              |
| 22:b:6019:CLA:HHC  | 22:b:6019:CLA:HBB1 | 1.67                     | 0.75              |
| 3:c:5249:ILE:O     | 3:c:5252:ILE:HG22  | 1.86                     | 0.75              |
| 4:d:5246:MET:HE3   | 4:d:5264:LYS:CG    | 2.14                     | 0.75              |
| 5:e:5042:LEU:O     | 5:e:5046:VAL:HG23  | 1.86                     | 0.75              |
| 7:h:5041:PHE:CZ    | 7:h:5045:ILE:HD11  | 2.22                     | 0.75              |
| 15:u:5063:ASN:CG   | 15:u:5063:ASN:O    | 2.30                     | 0.75              |
| 16:v:5151:ILE:HD13 | 16:v:5151:ILE:H    | 1.51                     | 0.75              |
| 1:A:225:ARG:O      | 1:A:226:GLU:HB2    | 1.87                     | 0.75              |
| 22:A:1006:CLA:HBC1 | 4:D:182:LEU:HD21   | 1.68                     | 0.75              |
| 2:B:12:LEU:H       | 2:B:12:LEU:HD12    | 1.52                     | 0.75              |
| 2:B:384:ARG:HD3    | 15:U:102:LEU:HD21  | 1.69                     | 0.75              |
| 2:B:429:ILE:H      | 2:B:429:ILE:HD12   | 1.52                     | 0.75              |
| 22:C:1031:CLA:HAA1 | 22:C:1033:CLA:HED2 | 1.68                     | 0.75              |
| 7:H:41:PHE:CZ      | 7:H:45:ILE:HD11    | 2.22                     | 0.75              |
| 12:M:34:LYS:HG3    | 11:l:5009:PRO:CG   | 2.17                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:O:77:LEU:HD23   | 13:O:93:PRO:HA     | 1.69                     | 0.75              |
| 3:c:5056:HIS:HD2   | 3:c:5057:ALA:N     | 1.84                     | 0.75              |
| 3:c:5086:LEU:HD22  | 3:c:5089:ILE:HB    | 1.69                     | 0.75              |
| 3:c:5284:PHE:HB3   | 29:c:6055:DGD:HB71 | 1.69                     | 0.75              |
| 22:c:6033:CLA:CED  | 22:c:6033:CLA:OBD  | 2.35                     | 0.75              |
| 1:A:126:TYR:HD2    | 1:A:126:TYR:O      | 1.69                     | 0.75              |
| 2:B:149:LEU:HB2    | 22:B:1012:CLA:C20  | 2.17                     | 0.75              |
| 3:C:46:SER:CB      | 3:C:141:GLU:CB     | 2.59                     | 0.75              |
| 3:C:86:LEU:HD22    | 3:C:89:ILE:HB      | 1.69                     | 0.75              |
| 8:I:14:PHE:HD1     | 8:I:14:PHE:C       | 1.95                     | 0.75              |
| 25:T:6046:BCR:H23C | 25:T:6046:BCR:H403 | 1.69                     | 0.75              |
| 22:B:1013:CLA:CMB  | 22:B:1014:CLA:H11  | 2.16                     | 0.75              |
| 22:B:1018:CLA:H18  | 22:B:1023:CLA:HMD2 | 1.69                     | 0.75              |
| 22:B:1021:CLA:CED  | 22:B:1021:CLA:O1A  | 2.34                     | 0.75              |
| 22:B:1021:CLA:H112 | 28:B:1060:MGE:CDA  | 2.17                     | 0.75              |
| 5:E:42:LEU:O       | 5:E:46:VAL:HG23    | 1.86                     | 0.75              |
| 13:O:80:GLU:O      | 13:O:82:PRO:CD     | 2.33                     | 0.75              |
| 22:a:6007:CLA:HED2 | 22:a:6007:CLA:CAD  | 2.15                     | 0.75              |
| 23:a:6038:PHO:CMB  | 22:d:6005:CLA:H52  | 2.17                     | 0.75              |
| 2:b:5027:THR:HG23  | 22:b:6013:CLA:HBC1 | 1.69                     | 0.75              |
| 22:b:6009:CLA:HBA1 | 22:b:6009:CLA:CHA  | 2.15                     | 0.75              |
| 22:b:6009:CLA:OBD  | 22:b:6010:CLA:HBB2 | 1.87                     | 0.75              |
| 7:h:5053:LEU:HD12  | 7:h:5055:LEU:HD21  | 1.67                     | 0.75              |
| 8:i:5014:PHE:HD1   | 8:i:5014:PHE:C     | 1.95                     | 0.75              |
| 22:A:1007:CLA:C4   | 22:C:1029:CLA:C19  | 2.64                     | 0.75              |
| 22:A:1007:CLA:HBA2 | 22:A:1007:CLA:CBD  | 2.17                     | 0.75              |
| 2:B:191:ASN:ND2    | 7:H:60:VAL:HA      | 2.02                     | 0.75              |
| 22:K:1034:CLA:C4D  | 22:K:1034:CLA:H12  | 2.17                     | 0.75              |
| 13:O:82:PRO:HG3    | 13:O:89:ALA:HB1    | 1.68                     | 0.75              |
| 15:U:31:ASN:HD22   | 15:U:32:ILE:H      | 1.35                     | 0.75              |
| 22:b:6009:CLA:H3A  | 25:h:6049:BCR:H372 | 1.67                     | 0.75              |
| 4:d:5184:PHE:HE2   | 4:d:5188:PHE:CD1   | 2.03                     | 0.75              |
| 22:d:6004:CLA:HBB1 | 22:d:6004:CLA:CHC  | 2.15                     | 0.75              |
| 5:e:5013:ILE:HA    | 5:e:5016:SER:CB    | 2.16                     | 0.75              |
| 10:k:5032:PHE:O    | 10:k:5033:PHE:C    | 2.29                     | 0.75              |
| 2:B:463:PHE:CG     | 29:B:1058:DGD:HAV1 | 2.22                     | 0.74              |
| 22:B:1009:CLA:HBA1 | 22:B:1009:CLA:CBD  | 2.15                     | 0.74              |
| 22:C:1033:CLA:HMA3 | 22:K:1034:CLA:CMC  | 2.16                     | 0.74              |
| 22:a:6007:CLA:C4   | 22:c:6029:CLA:C19  | 2.64                     | 0.74              |
| 22:a:6007:CLA:HBA2 | 22:a:6007:CLA:CBD  | 2.17                     | 0.74              |
| 2:b:5121:GLU:HB2   | 7:h:5004:ARG:HB3   | 1.69                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6009:CLA:CED  | 22:b:6009:CLA:C2A  | 2.53                     | 0.74              |
| 22:b:6023:CLA:C9   | 22:b:6024:CLA:C15  | 2.65                     | 0.74              |
| 4:d:5118:GLY:HA3   | 23:d:6039:PHO:H8   | 1.69                     | 0.74              |
| 1:A:293:MET:HG2    | 1:A:298:ASN:HA     | 1.68                     | 0.74              |
| 22:B:1013:CLA:CAB  | 22:B:1014:CLA:H51  | 2.17                     | 0.74              |
| 22:C:1029:CLA:HMD2 | 22:C:1031:CLA:HAB  | 1.69                     | 0.74              |
| 22:C:1031:CLA:HBC2 | 22:C:1031:CLA:CHD  | 2.11                     | 0.74              |
| 4:D:118:GLY:CA     | 23:D:1039:PHO:H8   | 2.16                     | 0.74              |
| 8:I:14:PHE:HE1     | 8:I:18:LEU:HD12    | 1.52                     | 0.74              |
| 1:a:5013:LEU:H     | 1:a:5013:LEU:HD12  | 1.51                     | 0.74              |
| 1:a:5180:PHE:CE1   | 4:d:5192:THR:HB    | 2.22                     | 0.74              |
| 1:a:5210:LEU:HD23  | 1:a:5210:LEU:C     | 2.11                     | 0.74              |
| 1:a:5219:VAL:HG11  | 4:d:5268:HIS:CG    | 2.22                     | 0.74              |
| 2:b:5053:ASN:N     | 2:b:5054:PRO:HD3   | 2.02                     | 0.74              |
| 22:c:6025:CLA:HBB1 | 22:c:6025:CLA:HMB3 | 1.69                     | 0.74              |
| 8:i:5014:PHE:HE1   | 8:i:5018:LEU:HD12  | 1.51                     | 0.74              |
| 1:A:339:PHE:HB3    | 3:C:313:GLN:OE1    | 1.87                     | 0.74              |
| 22:B:1009:CLA:HBA1 | 22:B:1009:CLA:CHA  | 2.15                     | 0.74              |
| 3:C:263:ALA:C      | 3:C:264:PHE:HD2    | 1.95                     | 0.74              |
| 3:C:284:PHE:HB3    | 29:C:1055:DGD:HB71 | 1.69                     | 0.74              |
| 22:C:1035:CLA:HMD1 | 10:K:40:GLN:NE2    | 2.01                     | 0.74              |
| 4:D:191:TRP:NE1    | 4:D:197:HIS:CD2    | 2.55                     | 0.74              |
| 7:H:17:GLU:HB2     | 7:H:20:LYS:HB2     | 1.67                     | 0.74              |
| 22:K:1034:CLA:C4   | 22:K:1034:CLA:O2A  | 2.33                     | 0.74              |
| 26:a:6063:LHG:C38  | 26:a:6063:LHG:C34  | 2.40                     | 0.74              |
| 2:b:5429:ILE:HD12  | 2:b:5429:ILE:H     | 1.52                     | 0.74              |
| 22:b:6009:CLA:HAA1 | 25:h:6049:BCR:H363 | 1.66                     | 0.74              |
| 3:c:5283:GLY:HA3   | 22:c:6026:CLA:HBC3 | 1.69                     | 0.74              |
| 22:k:6034:CLA:H12  | 22:k:6034:CLA:C4D  | 2.17                     | 0.74              |
| 13:o:5129:PHE:HD2  | 13:o:5129:PHE:O    | 1.71                     | 0.74              |
| 1:A:13:LEU:H       | 1:A:13:LEU:HD12    | 1.51                     | 0.74              |
| 1:A:16:ARG:HA      | 1:A:19:ASN:ND2     | 2.02                     | 0.74              |
| 1:A:180:PHE:CE1    | 4:D:192:THR:HB     | 2.22                     | 0.74              |
| 2:B:12:LEU:HD12    | 2:B:12:LEU:N       | 2.02                     | 0.74              |
| 22:B:1018:CLA:HBB1 | 22:B:1018:CLA:CHC  | 2.14                     | 0.74              |
| 22:B:1023:CLA:C9   | 22:B:1024:CLA:C15  | 2.65                     | 0.74              |
| 3:C:32:GLY:HA3     | 3:C:41:ARG:CD      | 2.17                     | 0.74              |
| 22:a:6007:CLA:H112 | 22:a:6007:CLA:H51  | 1.68                     | 0.74              |
| 22:b:6018:CLA:H18  | 22:b:6023:CLA:HMD2 | 1.69                     | 0.74              |
| 3:c:5049:LEU:CG    | 22:c:6035:CLA:HMA3 | 2.18                     | 0.74              |
| 22:c:6030:CLA:HHD  | 22:c:6030:CLA:HBC3 | 1.69                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:210:LEU:HD23   | 1:A:210:LEU:C      | 2.11                     | 0.74              |
| 22:B:1020:CLA:H11  | 22:B:1023:CLA:O1A  | 1.87                     | 0.74              |
| 7:H:33:VAL:O       | 7:H:37:LEU:HB2     | 1.87                     | 0.74              |
| 10:K:33:PHE:HB2    | 22:K:1034:CLA:H3A  | 1.68                     | 0.74              |
| 22:b:6021:CLA:H112 | 28:b:6060:MGE:CDA  | 2.17                     | 0.74              |
| 3:c:5109:PHE:HB3   | 3:c:5110:PRO:HD3   | 1.68                     | 0.74              |
| 13:o:5190:LEU:HD23 | 13:o:5190:LEU:C    | 2.12                     | 0.74              |
| 1:A:156:ALA:CA     | 1:A:160:ILE:HD12   | 2.17                     | 0.74              |
| 22:B:1022:CLA:H202 | 22:B:1022:CLA:CMD  | 2.18                     | 0.74              |
| 4:D:118:GLY:HA3    | 23:D:1039:PHO:H8   | 1.69                     | 0.74              |
| 2:b:5005:TRP:CD1   | 2:b:5005:TRP:H     | 2.05                     | 0.74              |
| 3:c:5112:PHE:O     | 3:c:5116:VAL:HG23  | 1.87                     | 0.74              |
| 3:c:5428:THR:CG2   | 3:c:5429:SER:H     | 2.01                     | 0.74              |
| 22:c:6025:CLA:C14  | 22:c:6031:CLA:HMB3 | 2.11                     | 0.74              |
| 4:d:5036:LEU:HD21  | 4:d:5124:GLY:CA    | 2.18                     | 0.74              |
| 4:d:5074:LEU:HD23  | 4:d:5175:VAL:HG11  | 1.70                     | 0.74              |
| 1:A:156:ALA:HA     | 1:A:160:ILE:CD1    | 2.16                     | 0.74              |
| 1:A:193:LEU:HD13   | 4:D:179:PHE:HB3    | 1.70                     | 0.74              |
| 24:A:1043:PQ9:H352 | 4:D:45:LEU:HD22    | 1.69                     | 0.74              |
| 3:C:49:LEU:CG      | 22:C:1035:CLA:HMA2 | 2.18                     | 0.74              |
| 3:C:437:PHE:HA     | 22:C:1032:CLA:CMC  | 2.18                     | 0.74              |
| 1:a:5224:ILE:N     | 2:b:5482:ILE:HG23  | 2.01                     | 0.74              |
| 2:b:5463:PHE:CG    | 29:b:6058:DGD:HAV1 | 2.22                     | 0.74              |
| 22:b:6013:CLA:CAB  | 22:b:6014:CLA:H51  | 2.17                     | 0.74              |
| 3:c:5237:HIS:O     | 3:c:5240:ILE:HG22  | 1.88                     | 0.74              |
| 29:c:6055:DGD:HB1  | 29:c:6055:DGD:HBG3 | 1.69                     | 0.74              |
| 4:d:5032:TRP:CE3   | 4:d:5032:TRP:HA    | 2.23                     | 0.74              |
| 4:d:5191:TRP:NE1   | 4:d:5197:HIS:CD2   | 2.55                     | 0.74              |
| 22:C:1033:CLA:CED  | 22:C:1033:CLA:OBD  | 2.35                     | 0.74              |
| 4:D:74:LEU:HD23    | 4:D:175:VAL:HG11   | 1.70                     | 0.74              |
| 22:a:6007:CLA:H43  | 22:c:6029:CLA:H191 | 1.68                     | 0.74              |
| 22:b:6022:CLA:H202 | 22:b:6022:CLA:CMD  | 2.18                     | 0.74              |
| 24:d:6042:PQ9:H242 | 28:l:6061:MGE:H263 | 1.70                     | 0.74              |
| 13:o:5077:LEU:HD23 | 13:o:5093:PRO:HA   | 1.69                     | 0.74              |
| 3:C:472:LEU:O      | 3:C:473:ASP:HB2    | 1.85                     | 0.74              |
| 22:C:1028:CLA:H93  | 29:C:1056:DGD:HB61 | 1.70                     | 0.74              |
| 7:H:53:LEU:HD12    | 7:H:55:LEU:HD21    | 1.67                     | 0.74              |
| 13:O:190:LEU:HD23  | 13:O:190:LEU:C     | 2.12                     | 0.74              |
| 2:b:5385:ARG:HD3   | 15:u:5014:ASP:OD2  | 1.87                     | 0.74              |
| 22:b:6009:CLA:HAA2 | 25:h:6049:BCR:H372 | 1.70                     | 0.74              |
| 28:b:6060:MGE:H3B2 | 28:b:6060:MGE:C7B  | 2.17                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5437:PHE:HA    | 22:c:6032:CLA:CMC  | 2.18                     | 0.74              |
| 22:k:6034:CLA:HBC3 | 22:k:6034:CLA:CHD  | 2.16                     | 0.74              |
| 2:B:5:TRP:H        | 2:B:5:TRP:CD1      | 2.05                     | 0.74              |
| 2:B:12:LEU:O       | 2:B:14:ASN:N       | 2.21                     | 0.74              |
| 2:B:53:ASN:N       | 2:B:54:PRO:HD3     | 2.02                     | 0.74              |
| 3:C:349:ILE:HG22   | 3:C:375:LEU:HB2    | 1.68                     | 0.74              |
| 3:C:417:VAL:CG1    | 16:V:68:VAL:CG1    | 2.65                     | 0.74              |
| 13:O:129:PHE:HD2   | 13:O:129:PHE:O     | 1.71                     | 0.74              |
| 1:a:5040:THR:HG21  | 1:a:5122:GLY:H     | 1.53                     | 0.74              |
| 22:a:6007:CLA:HBA2 | 22:a:6007:CLA:CHA  | 2.18                     | 0.74              |
| 22:b:6009:CLA:CBD  | 22:b:6010:CLA:HBB2 | 1.97                     | 0.74              |
| 22:b:6019:CLA:H193 | 22:b:6021:CLA:H72  | 1.70                     | 0.74              |
| 3:c:5369:LEU:HD13  | 3:c:5380:ILE:HD12  | 1.70                     | 0.74              |
| 22:c:6028:CLA:H93  | 29:c:6056:DGD:HB61 | 1.70                     | 0.74              |
| 2:B:135:LEU:H      | 2:B:135:LEU:HD12   | 1.53                     | 0.73              |
| 2:B:156:PHE:O      | 2:B:162:PHE:HB3    | 1.88                     | 0.73              |
| 22:B:1023:CLA:O1D  | 22:B:1024:CLA:HBB2 | 1.88                     | 0.73              |
| 15:U:43:PRO:HG3    | 16:V:109:ASP:CA    | 2.17                     | 0.73              |
| 24:a:6043:PQ9:H352 | 4:d:5045:LEU:HD22  | 1.69                     | 0.73              |
| 2:b:5475:PHE:HD1   | 4:d:5140:PRO:HD3   | 1.53                     | 0.73              |
| 22:b:6016:CLA:H52  | 22:h:6017:CLA:H112 | 1.63                     | 0.73              |
| 23:d:6039:PHO:CMA  | 22:d:6004:CLA:H142 | 2.18                     | 0.73              |
| 13:o:5168:PHE:HB2  | 13:o:5225:LEU:HB2  | 1.69                     | 0.73              |
| 15:u:5043:PRO:HG3  | 16:v:5109:ASP:CA   | 2.17                     | 0.73              |
| 2:B:307:GLU:OE2    | 13:o:5085:LYS:HB3  | 1.87                     | 0.73              |
| 2:B:475:PHE:HD1    | 4:D:140:PRO:HD3    | 1.53                     | 0.73              |
| 22:B:1011:CLA:HED2 | 22:B:1012:CLA:HED2 | 1.61                     | 0.73              |
| 3:C:89:ILE:HG12    | 3:C:111:PHE:CD2    | 2.23                     | 0.73              |
| 3:C:428:THR:CG2    | 3:C:429:SER:H      | 2.01                     | 0.73              |
| 22:C:1033:CLA:HMA2 | 22:K:1034:CLA:C3C  | 2.17                     | 0.73              |
| 22:C:1033:CLA:CMA  | 22:K:1034:CLA:HAC1 | 2.16                     | 0.73              |
| 4:D:36:LEU:HD21    | 4:D:124:GLY:CA     | 2.18                     | 0.73              |
| 13:O:231:ASP:HB3   | 13:O:234:THR:OG1   | 1.88                     | 0.73              |
| 1:a:5156:ALA:HA    | 1:a:5160:ILE:CD1   | 2.16                     | 0.73              |
| 26:a:6063:LHG:H341 | 26:a:6063:LHG:H383 | 0.79                     | 0.73              |
| 2:b:5149:LEU:HB2   | 22:b:6012:CLA:C20  | 2.17                     | 0.73              |
| 3:c:5348:GLU:CG    | 3:c:5349:ILE:HG13  | 2.18                     | 0.73              |
| 22:c:6033:CLA:HMA2 | 22:k:6034:CLA:C3C  | 2.17                     | 0.73              |
| 7:h:5033:VAL:O     | 7:h:5037:LEU:HB2   | 1.87                     | 0.73              |
| 16:v:5038:LEU:HB2  | 16:v:5045:ILE:HD11 | 1.70                     | 0.73              |
| 1:A:116:ILE:HG23   | 1:A:117:PHE:N      | 2.04                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:A:1063:LHG:H322 | 22:K:1034:CLA:H13  | 1.70                     | 0.73              |
| 3:C:112:PHE:O      | 3:C:116:VAL:HG23   | 1.87                     | 0.73              |
| 29:C:1055:DGD:HBF1 | 29:C:1055:DGD:HGB3 | 1.69                     | 0.73              |
| 5:E:37:PHE:CE1     | 5:E:46:VAL:HG21    | 2.23                     | 0.73              |
| 13:O:198:ILE:HG23  | 13:O:199:ALA:H     | 1.53                     | 0.73              |
| 1:a:5016:ARG:HA    | 1:a:5019:ASN:ND2   | 2.02                     | 0.73              |
| 3:c:5116:VAL:HG11  | 25:z:6053:BCR:HC31 | 1.70                     | 0.73              |
| 3:c:5397:THR:OG1   | 3:c:5398:HIS:N     | 2.13                     | 0.73              |
| 22:c:6030:CLA:HMB3 | 22:c:6031:CLA:NC   | 2.03                     | 0.73              |
| 4:d:5191:TRP:NE1   | 4:d:5197:HIS:HD2   | 1.85                     | 0.73              |
| 7:h:5048:ILE:HA    | 7:h:5053:LEU:HB3   | 1.70                     | 0.73              |
| 16:v:5092:ARG:HH11 | 16:v:5092:ARG:CG   | 2.02                     | 0.73              |
| 2:B:249:ALA:CB     | 2:B:459:ALA:HB2    | 2.19                     | 0.73              |
| 22:B:1021:CLA:CED  | 22:B:1021:CLA:CHA  | 2.61                     | 0.73              |
| 22:B:1023:CLA:C4C  | 22:B:1024:CLA:CBC  | 2.66                     | 0.73              |
| 28:B:1060:MGE:H212 | 28:B:1060:MGE:H251 | 0.79                     | 0.73              |
| 3:C:237:HIS:O      | 3:C:240:ILE:HG22   | 1.88                     | 0.73              |
| 16:V:46:THR:O      | 16:V:47:LEU:HB2    | 1.88                     | 0.73              |
| 2:b:5012:LEU:HD12  | 2:b:5012:LEU:H     | 1.52                     | 0.73              |
| 2:b:5213:GLY:O     | 2:b:5217:ILE:HG13  | 1.89                     | 0.73              |
| 22:b:6022:CLA:HBC2 | 22:b:6022:CLA:CHD  | 2.13                     | 0.73              |
| 22:b:6023:CLA:O1D  | 22:b:6024:CLA:HBB2 | 1.88                     | 0.73              |
| 3:c:5089:ILE:HG12  | 3:c:5111:PHE:CD2   | 2.23                     | 0.73              |
| 22:k:6034:CLA:C4   | 22:k:6034:CLA:O2A  | 2.33                     | 0.73              |
| 22:A:1007:CLA:H51  | 22:A:1007:CLA:H112 | 1.68                     | 0.73              |
| 2:B:385:ARG:HD3    | 15:U:14:ASP:OD2    | 1.87                     | 0.73              |
| 3:C:46:SER:OG      | 3:C:141:GLU:HB2    | 1.89                     | 0.73              |
| 3:C:146:PHE:CG     | 3:C:146:PHE:O      | 2.40                     | 0.73              |
| 3:C:164:HIS:HA     | 3:C:167:VAL:HB     | 1.71                     | 0.73              |
| 2:b:5156:PHE:O     | 2:b:5162:PHE:HB3   | 1.88                     | 0.73              |
| 22:b:6009:CLA:H121 | 22:b:6009:CLA:H91  | 0.83                     | 0.73              |
| 22:b:6022:CLA:H93  | 22:b:6022:CLA:C12  | 2.09                     | 0.73              |
| 14:t:5003:THR:HA   | 14:t:5006:TYR:HD2  | 1.53                     | 0.73              |
| 1:A:40:THR:HG21    | 1:A:122:GLY:H      | 1.53                     | 0.73              |
| 1:A:215:HIS:CE1    | 1:A:271:LEU:HD11   | 2.24                     | 0.73              |
| 22:A:1006:CLA:H93  | 22:D:1004:CLA:H152 | 1.71                     | 0.73              |
| 22:A:1007:CLA:HBA2 | 22:A:1007:CLA:CHA  | 2.18                     | 0.73              |
| 2:B:27:THR:HG23    | 22:B:1013:CLA:CBC  | 2.18                     | 0.73              |
| 2:B:121:GLU:HB2    | 7:H:4:ARG:HB3      | 1.69                     | 0.73              |
| 2:B:475:PHE:CD1    | 4:D:140:PRO:HD3    | 2.24                     | 0.73              |
| 22:B:1022:CLA:HBC2 | 22:B:1022:CLA:CHD  | 2.13                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:H:48:ILE:HA      | 7:H:53:LEU:HB3     | 1.71                     | 0.73              |
| 1:a:5193:LEU:HD13  | 4:d:5179:PHE:HB3   | 1.70                     | 0.73              |
| 1:a:5225:ARG:O     | 1:a:5226:GLU:HB2   | 1.87                     | 0.73              |
| 22:a:6006:CLA:H93  | 22:d:6004:CLA:H152 | 1.71                     | 0.73              |
| 2:b:5012:LEU:HD12  | 2:b:5012:LEU:N     | 2.02                     | 0.73              |
| 2:b:5357:ARG:HG2   | 2:b:5357:ARG:HH11  | 1.53                     | 0.73              |
| 2:b:5392:PHE:HA    | 2:b:5397:VAL:HG23  | 1.68                     | 0.73              |
| 22:b:6011:CLA:HBB1 | 22:b:6011:CLA:C9   | 2.19                     | 0.73              |
| 3:c:5049:LEU:CD1   | 3:c:5049:LEU:N     | 2.51                     | 0.73              |
| 3:c:5146:PHE:CG    | 3:c:5146:PHE:O     | 2.40                     | 0.73              |
| 7:h:5029:PRO:O     | 7:h:5033:VAL:HG13  | 1.89                     | 0.73              |
| 1:A:202:VAL:HG11   | 22:A:1006:CLA:OBD  | 1.89                     | 0.73              |
| 2:B:27:THR:HG23    | 22:B:1013:CLA:HBC1 | 1.69                     | 0.73              |
| 2:B:159:THR:HA     | 2:B:181:VAL:O      | 1.89                     | 0.73              |
| 22:B:1019:CLA:C9   | 28:L:1061:MGE:H9A2 | 2.18                     | 0.73              |
| 3:C:167:VAL:HG13   | 22:C:1036:CLA:H42  | 1.69                     | 0.73              |
| 22:C:1030:CLA:HMB3 | 22:C:1031:CLA:NC   | 2.03                     | 0.73              |
| 22:D:1005:CLA:CBC  | 22:D:1004:CLA:CBB  | 2.64                     | 0.73              |
| 7:H:31:MET:SD      | 22:H:1017:CLA:HAA1 | 2.29                     | 0.73              |
| 1:a:5246:TYR:H     | 1:a:5246:TYR:HD1   | 1.34                     | 0.73              |
| 25:b:6047:BCR:H331 | 25:b:6047:BCR:C8   | 2.14                     | 0.73              |
| 3:c:5187:ASP:HB2   | 3:c:5230:LEU:HD11  | 1.70                     | 0.73              |
| 3:c:5334:PRO:HA    | 13:o:5179:THR:OG1  | 1.89                     | 0.73              |
| 22:c:6029:CLA:HMD2 | 22:c:6031:CLA:HAB  | 1.69                     | 0.73              |
| 1:A:205:VAL:HB     | 1:A:279:ARG:NH2    | 2.04                     | 0.73              |
| 23:A:1038:PHO:CMB  | 22:D:1005:CLA:H52  | 2.17                     | 0.73              |
| 25:A:1044:BCR:H331 | 25:A:1044:BCR:C8   | 2.19                     | 0.73              |
| 3:C:179:ALA:CB     | 3:C:199:ILE:HD13   | 2.19                     | 0.73              |
| 3:C:287:THR:HG21   | 3:C:431:PHE:HB2    | 1.71                     | 0.73              |
| 22:C:1030:CLA:HBB2 | 22:C:1031:CLA:CED  | 2.16                     | 0.73              |
| 4:D:32:TRP:HA      | 4:D:32:TRP:CE3     | 2.23                     | 0.73              |
| 16:V:38:LEU:HB2    | 16:V:45:ILE:HD11   | 1.70                     | 0.73              |
| 22:b:6018:CLA:HBB1 | 22:b:6018:CLA:CHC  | 2.14                     | 0.73              |
| 22:b:6020:CLA:H11  | 22:b:6023:CLA:O1A  | 1.87                     | 0.73              |
| 3:c:5263:ALA:HB3   | 3:c:5264:PHE:HE2   | 1.48                     | 0.73              |
| 6:f:5036:ALA:O     | 6:f:5039:ALA:HB3   | 1.89                     | 0.73              |
| 22:K:1034:CLA:H102 | 22:K:1034:CLA:C14  | 2.13                     | 0.73              |
| 2:b:5354:LEU:C     | 2:b:5355:PHE:HD2   | 1.97                     | 0.73              |
| 2:B:25:MET:C       | 2:B:27:THR:N       | 2.44                     | 0.73              |
| 3:C:187:ASP:HB2    | 3:C:230:LEU:HD11   | 1.70                     | 0.73              |
| 3:C:369:LEU:HD13   | 3:C:380:ILE:HD12   | 1.70                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1030:CLA:HHD  | 22:C:1030:CLA:HBC3 | 1.69                     | 0.73              |
| 11:L:9:PRO:CG      | 12:m:5034:LYS:HG3  | 2.19                     | 0.73              |
| 14:T:3:THR:HA      | 14:T:6:TYR:HD2     | 1.53                     | 0.73              |
| 15:U:42:TYR:CD2    | 15:U:43:PRO:N      | 2.57                     | 0.73              |
| 15:U:64:ILE:HB     | 15:U:67:LEU:HD11   | 1.70                     | 0.73              |
| 1:a:5279:ARG:NH2   | 23:a:6038:PHO:HMC2 | 1.99                     | 0.73              |
| 3:c:5263:ALA:C     | 3:c:5264:PHE:HD2   | 1.95                     | 0.73              |
| 4:d:5281:MET:HE2   | 4:d:5281:MET:HA    | 1.70                     | 0.73              |
| 2:B:172:TYR:O      | 2:B:174:LEU:CA     | 2.29                     | 0.72              |
| 2:B:357:ARG:HG2    | 2:B:357:ARG:HH11   | 1.53                     | 0.72              |
| 22:B:1009:CLA:HAA2 | 25:H:1049:BCR:H372 | 1.69                     | 0.72              |
| 3:C:140:LEU:HD23   | 3:C:140:LEU:O      | 1.88                     | 0.72              |
| 22:D:1005:CLA:C4A  | 22:D:1005:CLA:O1A  | 2.37                     | 0.72              |
| 3:c:5032:GLY:HA3   | 3:c:5041:ARG:CD    | 2.17                     | 0.72              |
| 3:c:5179:ALA:CB    | 3:c:5199:ILE:HD13  | 2.19                     | 0.72              |
| 5:e:5037:PHE:CE1   | 5:e:5046:VAL:HG21  | 2.23                     | 0.72              |
| 13:o:5198:ILE:HG23 | 13:o:5199:ALA:H    | 1.53                     | 0.72              |
| 25:t:1046:BCR:H392 | 25:t:1046:BCR:C23  | 2.17                     | 0.72              |
| 25:t:1046:BCR:H23C | 25:t:1046:BCR:H403 | 1.69                     | 0.72              |
| 22:B:1011:CLA:C9   | 22:B:1011:CLA:HBB1 | 2.19                     | 0.72              |
| 7:H:29:PRO:O       | 7:H:33:VAL:HG13    | 1.89                     | 0.72              |
| 7:H:56:ASP:O       | 7:H:58:VAL:HG23    | 1.89                     | 0.72              |
| 13:O:168:PHE:HB2   | 13:O:225:LEU:HB2   | 1.69                     | 0.72              |
| 16:V:92:ARG:HH11   | 16:V:92:ARG:CG     | 2.02                     | 0.72              |
| 1:a:5159:LEU:HD12  | 1:a:5159:LEU:O     | 1.90                     | 0.72              |
| 2:b:5144:PHE:CE1   | 2:b:5210:ILE:HG23  | 2.24                     | 0.72              |
| 22:b:6023:CLA:C4C  | 22:b:6024:CLA:CB   | 2.66                     | 0.72              |
| 25:b:6045:BCR:H361 | 25:b:6045:BCR:C37  | 2.19                     | 0.72              |
| 3:c:5343:ARG:HH12  | 3:c:5348:GLU:HG3   | 0.74                     | 0.72              |
| 7:h:5031:MET:SD    | 22:h:6017:CLA:HAA1 | 2.29                     | 0.72              |
| 26:A:1063:LHG:HC62 | 26:A:1063:LHG:O9   | 1.77                     | 0.72              |
| 2:B:220:ARG:CD     | 2:B:221:PRO:HD2    | 2.20                     | 0.72              |
| 22:B:1011:CLA:HBB1 | 22:B:1011:CLA:H92  | 1.71                     | 0.72              |
| 3:C:116:VAL:HG11   | 25:Z:1053:BCR:HC31 | 1.70                     | 0.72              |
| 4:D:65:SER:HB2     | 4:D:77:ALA:O       | 1.88                     | 0.72              |
| 4:D:191:TRP:NE1    | 4:D:197:HIS:HD2    | 1.85                     | 0.72              |
| 22:D:1005:CLA:HBC2 | 22:D:1005:CLA:HHD  | 1.71                     | 0.72              |
| 6:F:24:HIS:HE1     | 31:F:1040:HEM:NC   | 1.88                     | 0.72              |
| 25:T:6046:BCR:H392 | 25:T:6046:BCR:C23  | 2.17                     | 0.72              |
| 2:b:5249:ALA:CB    | 2:b:5459:ALA:HB2   | 2.19                     | 0.72              |
| 3:c:5349:ILE:HG22  | 3:c:5375:LEU:HB2   | 1.68                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5065:SER:HB2   | 4:d:5077:ALA:O     | 1.88                     | 0.72              |
| 13:o:5231:ASP:HB3  | 13:o:5234:THR:OG1  | 1.88                     | 0.72              |
| 26:A:1063:LHG:C29  | 22:C:1032:CLA:H71  | 2.16                     | 0.72              |
| 2:B:144:PHE:CE1    | 2:B:210:ILE:HG23   | 2.24                     | 0.72              |
| 6:F:40:MET:O       | 6:F:42:PHE:N       | 2.22                     | 0.72              |
| 2:b:5103:LEU:HD11  | 2:b:5107:LEU:HD11  | 1.69                     | 0.72              |
| 2:b:5119:ASP:HB3   | 7:h:5003:ARG:HH21  | 1.54                     | 0.72              |
| 2:b:5121:GLU:HG3   | 7:h:5012:ARG:HD3   | 1.71                     | 0.72              |
| 2:b:5222:PRO:HB2   | 2:b:5225:LEU:CD1   | 2.20                     | 0.72              |
| 22:b:6011:CLA:O1D  | 22:b:6013:CLA:C1   | 2.35                     | 0.72              |
| 22:b:6021:CLA:O1A  | 22:b:6021:CLA:CGD  | 2.37                     | 0.72              |
| 3:c:5167:VAL:HG13  | 22:c:6036:CLA:H42  | 1.69                     | 0.72              |
| 3:c:5287:THR:HG23  | 3:c:5427:ALA:O     | 1.88                     | 0.72              |
| 16:v:5046:THR:O    | 16:v:5047:LEU:HB2  | 1.88                     | 0.72              |
| 22:B:1021:CLA:O1A  | 22:B:1021:CLA:CGD  | 2.37                     | 0.72              |
| 3:C:29:GLU:HA      | 3:C:41:ARG:NH1     | 2.04                     | 0.72              |
| 3:C:334:PRO:HA     | 13:O:179:THR:OG1   | 1.89                     | 0.72              |
| 3:C:348:GLU:CG     | 3:C:349:ILE:HG13   | 2.18                     | 0.72              |
| 24:D:1042:PQ9:H242 | 28:L:1061:MGE:H263 | 1.70                     | 0.72              |
| 5:E:20:TRP:CZ2     | 9:J:13:VAL:HG23    | 2.24                     | 0.72              |
| 7:H:12:ARG:NH1     | 7:H:15:ASN:HB3     | 2.03                     | 0.72              |
| 1:a:5215:HIS:CE1   | 1:a:5271:LEU:HD11  | 2.24                     | 0.72              |
| 2:b:5012:LEU:O     | 2:b:5014:ASN:N     | 2.21                     | 0.72              |
| 2:b:5159:THR:HA    | 2:b:5181:VAL:O     | 1.89                     | 0.72              |
| 3:c:5266:TRP:HE3   | 3:c:5271:TYR:HH    | 1.37                     | 0.72              |
| 7:h:5004:ARG:O     | 7:h:5005:THR:HG23  | 1.90                     | 0.72              |
| 15:u:5031:ASN:HD22 | 15:u:5032:ILE:H    | 1.35                     | 0.72              |
| 15:u:5042:TYR:CD2  | 15:u:5043:PRO:N    | 2.57                     | 0.72              |
| 18:y:5026:ALA:O    | 18:y:5030:ILE:HG22 | 1.90                     | 0.72              |
| 1:A:159:LEU:HD12   | 1:A:159:LEU:O      | 1.90                     | 0.72              |
| 2:B:121:GLU:HG3    | 7:H:12:ARG:HD3     | 1.71                     | 0.72              |
| 2:B:213:GLY:O      | 2:B:217:ILE:HG13   | 1.89                     | 0.72              |
| 3:C:287:THR:HG23   | 3:C:427:ALA:O      | 1.88                     | 0.72              |
| 22:C:1025:CLA:HBB1 | 22:C:1025:CLA:HMB3 | 1.69                     | 0.72              |
| 4:D:126:MET:HE2    | 4:D:146:PHE:HB3    | 1.71                     | 0.72              |
| 26:a:6063:LHG:H322 | 22:k:6034:CLA:H13  | 1.70                     | 0.72              |
| 2:b:5135:LEU:H     | 2:b:5135:LEU:HD12  | 1.53                     | 0.72              |
| 3:c:5046:SER:OG    | 3:c:5141:GLU:HB2   | 1.89                     | 0.72              |
| 22:d:6005:CLA:HBC2 | 22:d:6004:CLA:CBB  | 2.18                     | 0.72              |
| 6:f:5024:HIS:HE1   | 31:f:6040:HEM:NC   | 1.88                     | 0.72              |
| 22:A:1007:CLA:H43  | 22:C:1029:CLA:H191 | 1.68                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1019:CLA:H193 | 22:B:1021:CLA:H72  | 1.70                     | 0.72              |
| 3:C:400:PRO:C      | 3:C:401:LEU:HD22   | 2.15                     | 0.72              |
| 22:K:1034:CLA:H42  | 22:K:1034:CLA:O2A  | 1.89                     | 0.72              |
| 18:Y:26:ALA:O      | 18:Y:30:ILE:HG22   | 1.90                     | 0.72              |
| 22:b:6011:CLA:HBB1 | 22:b:6011:CLA:H92  | 1.72                     | 0.72              |
| 22:b:6012:CLA:CMB  | 22:b:6015:CLA:CBB  | 2.68                     | 0.72              |
| 3:c:5056:HIS:O     | 3:c:5058:GLY:N     | 2.23                     | 0.72              |
| 3:c:5140:LEU:O     | 3:c:5140:LEU:HD23  | 1.88                     | 0.72              |
| 17:x:5034:PHE:O    | 17:x:5038:ILE:HG12 | 1.90                     | 0.72              |
| 1:A:272:HIS:NE2    | 4:D:214:HIS:CE1    | 2.58                     | 0.72              |
| 2:B:12:LEU:HD22    | 2:B:19:LEU:CD1     | 2.20                     | 0.72              |
| 2:B:27:THR:OG1     | 22:B:1020:CLA:H43  | 1.90                     | 0.72              |
| 22:B:1009:CLA:OBD  | 22:B:1010:CLA:HBB2 | 1.87                     | 0.72              |
| 22:B:1021:CLA:C4   | 28:B:1060:MGE:H242 | 2.20                     | 0.72              |
| 4:D:68:LEU:HD23    | 5:E:49:THR:HG21    | 1.72                     | 0.72              |
| 6:F:36:ALA:O       | 6:F:39:ALA:HB3     | 1.89                     | 0.72              |
| 10:K:37:PHE:CB     | 25:K:1051:BCR:H401 | 2.19                     | 0.72              |
| 24:a:6043:PQ9:C45  | 28:d:6059:MGE:H8A2 | 2.20                     | 0.72              |
| 2:b:5012:LEU:HD22  | 2:b:5019:LEU:CD1   | 2.19                     | 0.72              |
| 22:b:6021:CLA:H112 | 28:b:6060:MGE:H132 | 1.72                     | 0.72              |
| 22:b:6021:CLA:C4   | 28:b:6060:MGE:H242 | 2.20                     | 0.72              |
| 3:c:5287:THR:HG21  | 3:c:5431:PHE:HB2   | 1.71                     | 0.72              |
| 3:c:5464:GLU:OE1   | 3:c:5467:LEU:HD12  | 1.90                     | 0.72              |
| 22:c:6029:CLA:O1A  | 22:c:6029:CLA:CBD  | 2.38                     | 0.72              |
| 29:c:6056:DGD:HAV1 | 29:c:6057:DGD:C8A  | 2.20                     | 0.72              |
| 16:v:5039:ASN:ND2  | 16:v:5040:SER:H    | 1.88                     | 0.72              |
| 22:A:1006:CLA:HBB1 | 22:A:1006:CLA:CHC  | 2.19                     | 0.72              |
| 2:B:176:GLY:HA3    | 2:B:266:GLU:OE2    | 1.90                     | 0.72              |
| 2:B:247:PHE:O      | 2:B:251:VAL:HG23   | 1.90                     | 0.72              |
| 2:B:354:LEU:C      | 2:B:355:PHE:HD2    | 1.97                     | 0.72              |
| 22:B:1012:CLA:CMB  | 22:B:1015:CLA:CBB  | 2.68                     | 0.72              |
| 22:B:1012:CLA:O1A  | 22:B:1020:CLA:H141 | 1.90                     | 0.72              |
| 3:C:461:ARG:HG3    | 4:D:225:ASP:OD2    | 1.90                     | 0.72              |
| 3:C:464:GLU:OE1    | 3:C:467:LEU:HD12   | 1.90                     | 0.72              |
| 22:C:1029:CLA:O1A  | 22:C:1029:CLA:CBD  | 2.38                     | 0.72              |
| 22:C:1030:CLA:C12  | 22:C:1030:CLA:C17  | 2.30                     | 0.72              |
| 4:D:53:THR:HA      | 4:D:67:TYR:CD2     | 2.25                     | 0.72              |
| 13:O:190:LEU:HD23  | 13:O:190:LEU:O     | 1.90                     | 0.72              |
| 16:V:159:GLY:O     | 16:V:161:VAL:N     | 2.23                     | 0.72              |
| 1:a:5272:HIS:CG    | 4:d:5218:VAL:HG11  | 2.24                     | 0.72              |
| 2:b:5027:THR:HG23  | 22:b:6013:CLA:CBC  | 2.18                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6023:CLA:H161 | 22:b:6023:CLA:C10  | 2.20                     | 0.72              |
| 28:b:6060:MGE:CBB  | 28:b:6060:MGE:CGB  | 2.68                     | 0.72              |
| 3:c:5461:ARG:HG3   | 4:d:5225:ASP:OD2   | 1.90                     | 0.72              |
| 22:d:6005:CLA:HBC2 | 22:d:6005:CLA:HHD  | 1.71                     | 0.72              |
| 12:m:5032:GLN:HA   | 12:m:5032:GLN:HE21 | 1.55                     | 0.72              |
| 15:u:5064:ILE:HB   | 15:u:5067:LEU:HD11 | 1.70                     | 0.72              |
| 22:B:1016:CLA:C5   | 22:H:1017:CLA:C9   | 2.34                     | 0.72              |
| 3:C:283:GLY:HA3    | 22:C:1026:CLA:HBC3 | 1.70                     | 0.72              |
| 1:a:5116:ILE:HG23  | 1:a:5117:PHE:N     | 2.04                     | 0.72              |
| 2:b:5125:ASP:HB3   | 2:b:5128:THR:OG1   | 1.88                     | 0.72              |
| 2:b:5144:PHE:HE1   | 2:b:5210:ILE:HG23  | 1.55                     | 0.72              |
| 22:c:6031:CLA:O1A  | 22:c:6033:CLA:H51  | 1.90                     | 0.72              |
| 4:d:5305:ALA:HB1   | 13:o:5186:LYS:HD2  | 1.71                     | 0.72              |
| 6:f:5040:MET:O     | 6:f:5042:PHE:N     | 2.22                     | 0.72              |
| 13:o:5045:CYS:H    | 13:o:5072:GLN:NE2  | 1.88                     | 0.72              |
| 15:u:5045:LEU:HD21 | 15:u:5075:LEU:CD1  | 2.19                     | 0.72              |
| 2:B:222:PRO:HD2    | 22:H:1017:CLA:O1D  | 1.90                     | 0.71              |
| 22:B:1023:CLA:H161 | 22:B:1023:CLA:C10  | 2.20                     | 0.71              |
| 4:D:299:ILE:O      | 4:D:301:GLN:N      | 2.23                     | 0.71              |
| 7:H:4:ARG:O        | 7:H:5:THR:HG23     | 1.90                     | 0.71              |
| 12:M:32:GLN:HA     | 12:M:32:GLN:HE21   | 1.55                     | 0.71              |
| 17:X:34:PHE:O      | 17:X:38:ILE:HG12   | 1.90                     | 0.71              |
| 1:a:5156:ALA:CA    | 1:a:5160:ILE:HD12  | 2.17                     | 0.71              |
| 22:c:6030:CLA:H43  | 25:c:6054:BCR:HC8  | 1.71                     | 0.71              |
| 22:c:6035:CLA:C8   | 25:k:6052:BCR:H403 | 2.10                     | 0.71              |
| 4:d:5018:LEU:O     | 4:d:5022:LEU:HG    | 1.90                     | 0.71              |
| 4:d:5053:THR:HA    | 4:d:5067:TYR:CD2   | 2.25                     | 0.71              |
| 4:d:5191:TRP:HE1   | 4:d:5197:HIS:HD2   | 1.36                     | 0.71              |
| 1:A:135:TYR:CE1    | 3:C:449:ARG:HG3    | 2.25                     | 0.71              |
| 26:A:1063:LHG:H321 | 22:K:1034:CLA:C15  | 2.21                     | 0.71              |
| 2:B:103:LEU:HD11   | 2:B:107:LEU:HD11   | 1.69                     | 0.71              |
| 2:B:222:PRO:HB2    | 2:B:225:LEU:CD1    | 2.20                     | 0.71              |
| 2:B:482:ILE:O      | 2:B:483:ASP:HB3    | 1.90                     | 0.71              |
| 4:D:18:LEU:O       | 4:D:22:LEU:HG      | 1.90                     | 0.71              |
| 15:U:45:LEU:HD21   | 15:U:75:LEU:CD1    | 2.19                     | 0.71              |
| 2:b:5009:HIS:HB2   | 22:b:6019:CLA:O1A  | 1.90                     | 0.71              |
| 3:c:5048:LYS:NZ    | 3:c:5133:ALA:O     | 2.23                     | 0.71              |
| 3:c:5092:ILE:H     | 3:c:5092:ILE:CD1   | 2.03                     | 0.71              |
| 4:d:5249:ALA:HB1   | 24:d:6042:PQ9:H63  | 1.72                     | 0.71              |
| 4:d:5299:ILE:O     | 4:d:5301:GLN:N     | 2.23                     | 0.71              |
| 7:h:5056:ASP:O     | 7:h:5058:VAL:HG23  | 1.89                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:124:SER:O      | 1:A:127:MET:HB3    | 1.89                     | 0.71              |
| 2:B:119:ASP:HB3    | 7:H:3:ARG:HH21     | 1.54                     | 0.71              |
| 2:B:192:PRO:HG3    | 7:H:49:TYR:CE1     | 2.25                     | 0.71              |
| 3:C:52:ALA:O       | 3:C:55:ALA:HB3     | 1.91                     | 0.71              |
| 4:D:281:MET:HE2    | 4:D:281:MET:HA     | 1.70                     | 0.71              |
| 14:T:3:THR:HA      | 14:T:6:TYR:CD2     | 2.25                     | 0.71              |
| 16:V:39:ASN:ND2    | 16:V:40:SER:H      | 1.88                     | 0.71              |
| 1:a:5124:SER:O     | 1:a:5127:MET:HB3   | 1.89                     | 0.71              |
| 26:a:6063:LHG:O9   | 26:a:6063:LHG:HC62 | 1.77                     | 0.71              |
| 22:b:6019:CLA:C9   | 28:l:6061:MGE:H9A2 | 2.18                     | 0.71              |
| 3:c:5400:PRO:C     | 3:c:5401:LEU:HD22  | 2.15                     | 0.71              |
| 22:c:6029:CLA:CMD  | 22:c:6031:CLA:CAB  | 2.69                     | 0.71              |
| 10:k:5024:VAL:CG2  | 18:y:5025:ILE:HG22 | 2.18                     | 0.71              |
| 1:A:301:ASN:ND2    | 3:C:407:VAL:HG11   | 2.05                     | 0.71              |
| 2:B:373:LYS:C      | 2:B:374:ASN:HD22   | 1.99                     | 0.71              |
| 22:B:1010:CLA:H172 | 29:B:1058:DGD:HA82 | 1.72                     | 0.71              |
| 22:B:1016:CLA:C3   | 22:H:1017:CLA:H91  | 2.21                     | 0.71              |
| 3:C:266:TRP:HE3    | 3:C:271:TYR:HH     | 1.37                     | 0.71              |
| 28:D:1062:MGE:O1A  | 28:D:1062:MGE:H3B2 | 1.89                     | 0.71              |
| 7:H:43:LEU:HD23    | 7:H:44:ILE:N       | 2.05                     | 0.71              |
| 22:a:6003:CLA:H43  | 23:a:6038:PHO:C2B  | 2.21                     | 0.71              |
| 25:a:6044:BCR:H331 | 25:a:6044:BCR:C8   | 2.19                     | 0.71              |
| 2:b:5040:TYR:CD1   | 2:b:5040:TYR:C     | 2.67                     | 0.71              |
| 2:b:5105:GLY:CA    | 25:b:6047:BCR:H402 | 2.19                     | 0.71              |
| 2:b:5373:LYS:C     | 2:b:5374:ASN:HD22  | 1.99                     | 0.71              |
| 2:b:5399:VAL:HG23  | 2:b:5417:VAL:HG13  | 1.72                     | 0.71              |
| 25:b:6045:BCR:C8   | 25:b:6045:BCR:C33  | 2.66                     | 0.71              |
| 22:c:6025:CLA:HHB  | 22:c:6025:CLA:C1   | 2.06                     | 0.71              |
| 10:k:5032:PHE:HZ   | 25:k:6052:BCR:C36  | 1.96                     | 0.71              |
| 28:B:1060:MGE:CBB  | 28:B:1060:MGE:CGB  | 2.68                     | 0.71              |
| 3:C:56:HIS:O       | 3:C:58:GLY:N       | 2.23                     | 0.71              |
| 22:C:1032:CLA:CHB  | 22:K:1034:CLA:HBB2 | 2.21                     | 0.71              |
| 13:O:45:CYS:H      | 13:O:72:GLN:NE2    | 1.88                     | 0.71              |
| 16:V:98:LEU:HD22   | 16:V:98:LEU:N      | 2.03                     | 0.71              |
| 1:a:5202:VAL:HG11  | 22:a:6006:CLA:OBD  | 1.89                     | 0.71              |
| 2:b:5016:PRO:HG2   | 2:b:5133:LEU:HD13  | 1.73                     | 0.71              |
| 13:o:5190:LEU:HD23 | 13:o:5190:LEU:O    | 1.90                     | 0.71              |
| 16:v:5159:GLY:O    | 16:v:5161:VAL:N    | 2.23                     | 0.71              |
| 3:C:48:LYS:NZ      | 3:C:133:ALA:O      | 2.23                     | 0.71              |
| 22:C:1025:CLA:C14  | 22:C:1031:CLA:HMB3 | 2.11                     | 0.71              |
| 18:Y:43:ARG:HH21   | 18:Y:44:GLY:HA3    | 1.56                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:b:5005:TRP:C     | 2:b:5008:VAL:HG13 | 2.15                     | 0.71              |
| 2:b:5475:PHE:CD1   | 4:d:5140:PRO:HD3  | 2.24                     | 0.71              |
| 3:c:5164:HIS:HA    | 3:c:5167:VAL:HB   | 1.71                     | 0.71              |
| 4:d:5032:TRP:HA    | 4:d:5032:TRP:HE3  | 1.55                     | 0.71              |
| 4:d:5126:MET:HE2   | 4:d:5146:PHE:HB3  | 1.71                     | 0.71              |
| 1:A:192:ILE:CD1    | 1:A:293:MET:HE1   | 2.20                     | 0.71              |
| 22:A:1003:CLA:H43  | 23:A:1038:PHO:C2B | 2.21                     | 0.71              |
| 2:B:5:TRP:C        | 2:B:8:VAL:HG13    | 2.15                     | 0.71              |
| 29:C:1056:DGD:HAV1 | 29:C:1057:DGD:C8A | 2.20                     | 0.71              |
| 4:D:191:TRP:HE1    | 4:D:197:HIS:HD2   | 1.36                     | 0.71              |
| 15:U:29:ASN:HD21   | 15:U:87:VAL:HA    | 1.55                     | 0.71              |
| 15:U:59:GLU:C      | 15:U:61:VAL:H     | 1.98                     | 0.71              |
| 2:b:5013:ILE:HG13  | 2:b:5014:ASN:N    | 2.06                     | 0.71              |
| 2:b:5098:LEU:HD13  | 2:b:5098:LEU:C    | 2.16                     | 0.71              |
| 2:b:5192:PRO:HG3   | 7:h:5049:TYR:CE1  | 2.25                     | 0.71              |
| 3:c:5346:THR:HB    | 13:o:5038:GLY:HA2 | 1.73                     | 0.71              |
| 22:c:6025:CLA:HED3 | 22:c:6025:CLA:CAD | 2.21                     | 0.71              |
| 4:d:5250:ASN:HB2   | 4:d:5260:ALA:CB   | 2.20                     | 0.71              |
| 22:d:6005:CLA:O1A  | 22:d:6005:CLA:C4A | 2.38                     | 0.71              |
| 13:o:5206:GLU:H    | 13:o:5206:GLU:CD  | 1.99                     | 0.71              |
| 15:u:5029:ASN:HD21 | 15:u:5087:VAL:HA  | 1.55                     | 0.71              |
| 2:B:98:LEU:HD13    | 2:B:98:LEU:C      | 2.16                     | 0.71              |
| 28:B:1060:MGE:H3B2 | 28:B:1060:MGE:C7B | 2.17                     | 0.71              |
| 3:C:92:ILE:H       | 3:C:92:ILE:CD1    | 2.03                     | 0.71              |
| 4:D:140:PRO:O      | 4:D:142:ASN:N     | 2.24                     | 0.71              |
| 4:D:315:TYR:CE2    | 4:D:319:LEU:HD12  | 2.25                     | 0.71              |
| 7:H:41:PHE:O       | 7:H:45:ILE:HG13   | 1.91                     | 0.71              |
| 1:a:5301:ASN:ND2   | 3:c:5407:VAL:HG11 | 2.06                     | 0.71              |
| 22:b:6020:CLA:C16  | 22:b:6020:CLA:C11 | 2.69                     | 0.71              |
| 3:c:5393:ALA:O     | 3:c:5397:THR:HG23 | 1.91                     | 0.71              |
| 28:d:6062:MGE:H2A2 | 14:t:5020:ALA:HB1 | 1.73                     | 0.71              |
| 5:e:5020:TRP:CZ2   | 9:j:5013:VAL:HG23 | 2.24                     | 0.71              |
| 7:h:5043:LEU:HD23  | 7:h:5044:ILE:N    | 2.05                     | 0.71              |
| 14:t:5003:THR:HA   | 14:t:5006:TYR:CD2 | 2.25                     | 0.71              |
| 2:B:125:ASP:HB3    | 2:B:128:THR:OG1   | 1.89                     | 0.71              |
| 3:C:117:VAL:HG12   | 3:C:118:HIS:H     | 1.56                     | 0.71              |
| 22:C:1030:CLA:H43  | 25:C:1054:BCR:HC8 | 1.71                     | 0.71              |
| 22:C:1031:CLA:O1A  | 22:C:1033:CLA:H51 | 1.90                     | 0.71              |
| 4:D:103:ARG:HD3    | 4:D:106:GLN:NE2   | 2.05                     | 0.71              |
| 4:D:305:ALA:HB1    | 13:O:186:LYS:HD2  | 1.71                     | 0.71              |
| 4:d:5315:TYR:CE2   | 4:d:5319:LEU:HD12 | 2.25                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:d:6062:MGE:H3B2 | 28:d:6062:MGE:O1A  | 1.89                     | 0.71              |
| 7:h:5035:MET:HA    | 25:h:6049:BCR:H331 | 1.73                     | 0.71              |
| 15:u:5045:LEU:HD21 | 15:u:5075:LEU:HD12 | 1.73                     | 0.71              |
| 26:A:1063:LHG:H341 | 26:A:1063:LHG:H383 | 0.79                     | 0.71              |
| 2:B:9:HIS:HB2      | 22:B:1019:CLA:O1A  | 1.90                     | 0.71              |
| 24:D:1042:PQ9:C39  | 28:L:1061:MGE:H241 | 2.21                     | 0.71              |
| 8:I:14:PHE:C       | 8:I:14:PHE:CD1     | 2.67                     | 0.71              |
| 22:K:1034:CLA:HBC3 | 22:K:1034:CLA:CHD  | 2.16                     | 0.71              |
| 13:O:206:GLU:CD    | 13:O:206:GLU:H     | 1.99                     | 0.71              |
| 2:b:5025:MET:C     | 2:b:5027:THR:N     | 2.44                     | 0.71              |
| 2:b:5329:PRO:O     | 2:b:5331:ASN:N     | 2.24                     | 0.71              |
| 3:c:5029:GLU:HA    | 3:c:5041:ARG:NH1   | 2.04                     | 0.71              |
| 3:c:5049:LEU:HB3   | 3:c:5133:ALA:CA    | 2.18                     | 0.71              |
| 22:c:6030:CLA:C4D  | 22:c:6030:CLA:CED  | 2.69                     | 0.71              |
| 29:c:6057:DGD:HD4  | 9:j:5038:SER:O     | 1.91                     | 0.71              |
| 4:d:5103:ARG:HD3   | 4:d:5106:GLN:NE2   | 2.05                     | 0.71              |
| 7:h:5044:ILE:O     | 7:h:5048:ILE:HG13  | 1.90                     | 0.71              |
| 22:k:6034:CLA:H42  | 22:k:6034:CLA:O2A  | 1.89                     | 0.71              |
| 12:m:5008:PHE:HE2  | 14:t:5001:MET:CG   | 2.04                     | 0.71              |
| 2:B:16:PRO:HG2     | 2:B:133:LEU:HD13   | 1.73                     | 0.70              |
| 3:C:275:SER:HB3    | 22:C:1033:CLA:HED3 | 1.72                     | 0.70              |
| 22:C:1025:CLA:OBD  | 22:C:1025:CLA:CED  | 2.32                     | 0.70              |
| 24:a:6043:PQ9:H212 | 23:d:6039:PHO:HED1 | 1.73                     | 0.70              |
| 2:b:5152:GLY:O     | 2:b:5156:PHE:HB2   | 1.90                     | 0.70              |
| 2:b:5284:ILE:HG23  | 2:b:5305:ILE:HD13  | 1.73                     | 0.70              |
| 1:A:45:THR:HG23    | 1:A:46:ILE:N       | 2.05                     | 0.70              |
| 24:A:1043:PQ9:C45  | 28:D:1059:MGE:H8A2 | 2.20                     | 0.70              |
| 22:B:1022:CLA:OBD  | 22:B:1022:CLA:HED2 | 1.90                     | 0.70              |
| 22:a:6006:CLA:C17  | 25:d:6050:BCR:C27  | 2.66                     | 0.70              |
| 2:b:5010:THR:O     | 2:b:5013:ILE:HG22  | 1.91                     | 0.70              |
| 2:b:5176:GLY:HA3   | 2:b:5266:GLU:OE2   | 1.90                     | 0.70              |
| 3:c:5284:PHE:HB3   | 29:c:6055:DGD:C7B  | 2.22                     | 0.70              |
| 3:c:5417:VAL:CG1   | 16:v:5068:VAL:CG1  | 2.65                     | 0.70              |
| 22:c:6025:CLA:OBD  | 22:c:6025:CLA:CED  | 2.32                     | 0.70              |
| 22:c:6032:CLA:CHB  | 22:k:6034:CLA:HBB2 | 2.21                     | 0.70              |
| 6:f:5045:ARG:HA    | 6:f:5045:ARG:NE    | 1.97                     | 0.70              |
| 7:h:5050:ASN:O     | 7:h:5051:SER:HB2   | 1.89                     | 0.70              |
| 2:B:122:LEU:HD21   | 7:H:11:LEU:C       | 2.16                     | 0.70              |
| 2:B:249:ALA:HB1    | 2:B:459:ALA:HB2    | 1.73                     | 0.70              |
| 22:B:1019:CLA:CHA  | 22:B:1019:CLA:CBA  | 2.69                     | 0.70              |
| 23:D:1039:PHO:CMA  | 22:D:1004:CLA:H142 | 2.18                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:H:44:ILE:O       | 7:H:48:ILE:HG13    | 1.90                     | 0.70              |
| 13:O:78:VAL:HG21   | 13:O:142:ILE:HG21  | 1.73                     | 0.70              |
| 13:O:214:LYS:HB3   | 13:O:251:MET:HB3   | 1.73                     | 0.70              |
| 1:a:5135:TYR:CE1   | 3:c:5449:ARG:HG3   | 2.25                     | 0.70              |
| 1:a:5140:ARG:NH1   | 1:a:5140:ARG:HB3   | 2.06                     | 0.70              |
| 10:k:5011:LEU:CD1  | 10:k:5022:VAL:HG21 | 2.21                     | 0.70              |
| 1:A:269:ARG:HD3    | 4:D:222:LEU:CD1    | 2.20                     | 0.70              |
| 1:A:272:HIS:CG     | 4:D:218:VAL:HG11   | 2.26                     | 0.70              |
| 24:A:1043:PQ9:H212 | 23:D:1039:PHO:HED1 | 1.73                     | 0.70              |
| 2:B:249:ALA:HB2    | 22:B:1012:CLA:HBC1 | 1.73                     | 0.70              |
| 3:C:188:THR:HG22   | 3:C:300:GLU:OE2    | 1.91                     | 0.70              |
| 3:C:346:THR:HB     | 13:O:38:GLY:HA2    | 1.73                     | 0.70              |
| 1:a:5339:PHE:HB3   | 1:a:5340:PRO:CD    | 2.21                     | 0.70              |
| 2:b:5027:THR:OG1   | 22:b:6020:CLA:H43  | 1.90                     | 0.70              |
| 22:b:6016:CLA:C3   | 22:h:6017:CLA:H91  | 2.21                     | 0.70              |
| 3:c:5282:MET:HA    | 3:c:5285:ILE:HD12  | 1.74                     | 0.70              |
| 4:d:5148:ALA:HB1   | 4:d:5279:LEU:CD1   | 2.22                     | 0.70              |
| 7:h:5017:GLU:HG3   | 7:h:5020:LYS:HE2   | 1.73                     | 0.70              |
| 7:h:5041:PHE:O     | 7:h:5045:ILE:HG13  | 1.91                     | 0.70              |
| 13:o:5076:PHE:HE2  | 13:o:5132:VAL:HG21 | 1.56                     | 0.70              |
| 13:o:5266:TYR:CD1  | 13:o:5267:ALA:N    | 2.60                     | 0.70              |
| 1:A:39:PRO:HA      | 1:A:42:LEU:HB2     | 1.73                     | 0.70              |
| 1:A:140:ARG:HB3    | 1:A:140:ARG:NH1    | 2.06                     | 0.70              |
| 1:A:324:ALA:HB2    | 4:D:329:MET:SD     | 2.32                     | 0.70              |
| 22:B:1020:CLA:C16  | 22:B:1020:CLA:C11  | 2.69                     | 0.70              |
| 3:C:348:GLU:OE2    | 3:C:349:ILE:HG13   | 1.92                     | 0.70              |
| 4:D:253:TRP:CA     | 4:D:256:ILE:HG22   | 2.15                     | 0.70              |
| 4:D:265:ARG:HG3    | 4:D:265:ARG:NH1    | 2.04                     | 0.70              |
| 6:F:22:ALA:O       | 6:F:24:HIS:N       | 2.25                     | 0.70              |
| 13:O:266:TYR:CD1   | 13:O:267:ALA:N     | 2.60                     | 0.70              |
| 1:a:5039:PRO:HA    | 1:a:5042:LEU:HB2   | 1.74                     | 0.70              |
| 1:a:5192:ILE:CD1   | 1:a:5293:MET:HE1   | 2.20                     | 0.70              |
| 1:a:5330:VAL:HG12  | 4:d:5348:ARG:HA    | 1.73                     | 0.70              |
| 26:a:6063:LHG:C29  | 22:c:6032:CLA:H71  | 2.21                     | 0.70              |
| 22:b:6022:CLA:OBD  | 22:b:6022:CLA:HED2 | 1.90                     | 0.70              |
| 22:b:6023:CLA:HMC3 | 22:b:6023:CLA:HBC2 | 1.73                     | 0.70              |
| 3:c:5088:LEU:HD11  | 22:c:6027:CLA:HBC2 | 1.74                     | 0.70              |
| 4:d:5068:LEU:HD23  | 5:e:5049:THR:HG21  | 1.72                     | 0.70              |
| 1:A:84:PRO:HA      | 1:A:112:TYR:CD1    | 2.26                     | 0.70              |
| 1:A:330:VAL:HG12   | 4:D:348:ARG:HA     | 1.73                     | 0.70              |
| 22:B:1011:CLA:C3D  | 22:B:1013:CLA:C2   | 2.70                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B:1045:BCR:H361 | 25:B:1045:BCR:C37  | 2.19                     | 0.70              |
| 22:C:1025:CLA:C1   | 22:C:1025:CLA:H3A  | 2.22                     | 0.70              |
| 4:D:50:THR:HG21    | 25:D:1050:BCR:H333 | 1.74                     | 0.70              |
| 2:b:5040:TYR:CE1   | 22:b:6015:CLA:HED1 | 2.26                     | 0.70              |
| 2:b:5092:SER:O     | 2:b:5094:GLU:N     | 2.24                     | 0.70              |
| 2:b:5222:PRO:HD2   | 22:h:6017:CLA:O1D  | 1.90                     | 0.70              |
| 2:b:5247:PHE:O     | 2:b:5251:VAL:HG23  | 1.90                     | 0.70              |
| 2:b:5475:PHE:HD2   | 2:b:5475:PHE:N     | 1.90                     | 0.70              |
| 22:b:6013:CLA:HAB  | 22:b:6014:CLA:H52  | 1.72                     | 0.70              |
| 22:b:6019:CLA:CHA  | 22:b:6019:CLA:CBA  | 2.69                     | 0.70              |
| 5:e:5057:ALA:HB3   | 5:e:5060:GLN:HG2   | 1.73                     | 0.70              |
| 13:o:5214:LYS:HB3  | 13:o:5251:MET:HB3  | 1.73                     | 0.70              |
| 16:v:5105:PRO:CG   | 16:v:5115:ALA:HA   | 2.21                     | 0.70              |
| 3:C:284:PHE:HB3    | 29:C:1055:DGD:C7B  | 2.22                     | 0.70              |
| 28:D:1062:MGE:H2A2 | 14:T:20:ALA:HB1    | 1.73                     | 0.70              |
| 7:H:50:ASN:O       | 7:H:51:SER:HB2     | 1.90                     | 0.70              |
| 10:K:11:LEU:CD1    | 10:K:22:VAL:HG21   | 2.21                     | 0.70              |
| 16:V:105:PRO:CG    | 16:V:115:ALA:HA    | 2.21                     | 0.70              |
| 1:a:5084:PRO:HA    | 1:a:5112:TYR:CD1   | 2.26                     | 0.70              |
| 22:a:6003:CLA:H71  | 22:a:6003:CLA:H43  | 1.67                     | 0.70              |
| 2:b:5172:TYR:HD2   | 2:b:5287:ARG:HH22  | 1.40                     | 0.70              |
| 22:b:6011:CLA:C3D  | 22:b:6013:CLA:C2   | 2.70                     | 0.70              |
| 3:c:5348:GLU:OE2   | 3:c:5349:ILE:HG13  | 1.92                     | 0.70              |
| 4:d:5140:PRO:O     | 4:d:5142:ASN:N     | 2.24                     | 0.70              |
| 24:d:6042:PQ9:C39  | 28:l:6061:MGE:H241 | 2.21                     | 0.70              |
| 5:e:5034:GLY:HA2   | 6:f:5032:PHE:HE1   | 1.56                     | 0.70              |
| 18:y:5045:ASN:HD22 | 18:y:5045:ASN:C    | 2.00                     | 0.70              |
| 26:A:1063:LHG:C38  | 26:A:1063:LHG:C34  | 2.40                     | 0.70              |
| 2:B:40:TYR:CE1     | 22:B:1015:CLA:HED1 | 2.26                     | 0.70              |
| 2:B:92:SER:O       | 2:B:94:GLU:N       | 2.24                     | 0.70              |
| 22:B:1014:CLA:HBC2 | 22:B:1014:CLA:CHD  | 2.11                     | 0.70              |
| 3:C:187:ASP:HB3    | 3:C:190:ALA:HB2    | 1.73                     | 0.70              |
| 3:C:282:MET:HA     | 3:C:285:ILE:HD12   | 1.74                     | 0.70              |
| 22:C:1029:CLA:H43  | 25:C:1054:BCR:C32  | 2.22                     | 0.70              |
| 4:D:209:LEU:HD22   | 24:D:1042:PQ9:H192 | 1.73                     | 0.70              |
| 2:b:5122:LEU:HD21  | 7:h:5011:LEU:C     | 2.15                     | 0.70              |
| 2:b:5482:ILE:O     | 2:b:5483:ASP:HB3   | 1.90                     | 0.70              |
| 3:c:5188:THR:HG22  | 3:c:5300:GLU:OE2   | 1.91                     | 0.70              |
| 3:c:5438:LEU:O     | 3:c:5438:LEU:HD13  | 1.92                     | 0.70              |
| 4:d:5050:THR:HG21  | 25:d:6050:BCR:H333 | 1.74                     | 0.70              |
| 22:k:6034:CLA:HHD  | 22:k:6034:CLA:CBC  | 2.17                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:212:CYS:O      | 4:D:271:MET:HB3    | 1.92                     | 0.70              |
| 2:B:40:TYR:C       | 2:B:40:TYR:CD1     | 2.67                     | 0.70              |
| 2:B:172:TYR:HD2    | 2:B:287:ARG:HH22   | 1.40                     | 0.70              |
| 2:B:329:PRO:O      | 2:B:331:ASN:N      | 2.24                     | 0.70              |
| 22:C:1030:CLA:CED  | 22:C:1030:CLA:C4D  | 2.69                     | 0.70              |
| 4:D:32:TRP:HA      | 4:D:32:TRP:HE3     | 1.55                     | 0.70              |
| 4:D:148:ALA:HB1    | 4:D:279:LEU:CD1    | 2.22                     | 0.70              |
| 4:D:329:MET:C      | 4:D:331:PRO:HD2    | 2.17                     | 0.70              |
| 22:D:1005:CLA:HBC2 | 22:D:1004:CLA:CBB  | 2.18                     | 0.70              |
| 5:E:37:PHE:HE1     | 5:E:46:VAL:HG21    | 1.56                     | 0.70              |
| 7:H:35:MET:HA      | 25:H:1049:BCR:H331 | 1.73                     | 0.70              |
| 2:b:5028:ALA:O     | 2:b:5104:SER:HB2   | 1.92                     | 0.70              |
| 2:b:5475:PHE:CD1   | 4:d:5140:PRO:CD    | 2.75                     | 0.70              |
| 4:d:5209:LEU:HD22  | 24:d:6042:PQ9:H192 | 1.73                     | 0.70              |
| 4:d:5265:ARG:HH11  | 4:d:5265:ARG:CG    | 2.03                     | 0.70              |
| 25:k:6051:BCR:C23  | 25:k:6051:BCR:C40  | 2.64                     | 0.70              |
| 18:y:5043:ARG:HH21 | 18:y:5044:GLY:HA3  | 1.56                     | 0.70              |
| 1:A:39:PRO:HD2     | 22:A:1007:CLA:HBB2 | 1.74                     | 0.70              |
| 2:B:323:GLY:HA3    | 2:B:326:ARG:HG3    | 1.74                     | 0.70              |
| 2:B:399:VAL:HG23   | 2:B:417:VAL:HG13   | 1.72                     | 0.70              |
| 22:B:1011:CLA:O1D  | 22:B:1013:CLA:C1   | 2.35                     | 0.70              |
| 22:B:1019:CLA:HMD2 | 28:B:1060:MGE:H1G1 | 1.74                     | 0.70              |
| 3:C:342:MET:SD     | 3:C:356:MET:HE2    | 2.32                     | 0.70              |
| 28:D:1062:MGE:O6D  | 11:L:15:THR:HG21   | 1.92                     | 0.70              |
| 13:O:215:ARG:HH11  | 13:O:215:ARG:HG2   | 1.57                     | 0.70              |
| 1:a:5045:THR:HG23  | 1:a:5046:ILE:N     | 2.05                     | 0.70              |
| 1:a:5124:SER:OG    | 1:a:5151:LEU:HD11  | 1.92                     | 0.70              |
| 3:c:5052:ALA:O     | 3:c:5055:ALA:HB3   | 1.91                     | 0.70              |
| 3:c:5187:ASP:HB3   | 3:c:5190:ALA:HB2   | 1.73                     | 0.70              |
| 22:d:6005:CLA:HAA2 | 24:d:6042:PQ9:H412 | 0.75                     | 0.70              |
| 11:l:5014:ARG:CA   | 12:m:5026:TYR:HE1  | 2.05                     | 0.70              |
| 16:v:5064:ALA:HB1  | 16:v:5068:VAL:HA   | 1.74                     | 0.70              |
| 1:A:272:HIS:CD2    | 4:D:214:HIS:CE1    | 2.80                     | 0.69              |
| 3:C:393:ALA:O      | 3:C:397:THR:HG23   | 1.91                     | 0.69              |
| 29:C:1057:DGD:HD4  | 9:J:38:SER:O       | 1.91                     | 0.69              |
| 4:D:249:ALA:HB1    | 24:D:1042:PQ9:H63  | 1.72                     | 0.69              |
| 7:H:14:LEU:HD12    | 7:H:14:LEU:H       | 1.57                     | 0.69              |
| 12:M:9:ILE:CG1     | 12:m:5008:PHE:HB3  | 2.21                     | 0.69              |
| 1:a:5324:ALA:HB2   | 4:d:5329:MET:SD    | 2.32                     | 0.69              |
| 2:b:5031:ALA:HB2   | 22:b:6013:CLA:HAC1 | 1.74                     | 0.69              |
| 2:b:5277:SER:O     | 2:b:5279:TYR:N     | 2.23                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:h:5012:ARG:NH1   | 7:h:5015:ASN:HB3   | 2.03                     | 0.69              |
| 12:m:5008:PHE:HE2  | 14:t:5001:MET:HG3  | 1.57                     | 0.69              |
| 13:o:5078:VAL:HG21 | 13:o:5142:ILE:HG21 | 1.73                     | 0.69              |
| 2:B:28:ALA:O       | 2:B:104:SER:HB2    | 1.92                     | 0.69              |
| 3:C:199:ILE:H      | 3:C:199:ILE:HD12   | 1.58                     | 0.69              |
| 3:C:450:ALA:CB     | 3:C:456:GLU:HB3    | 2.22                     | 0.69              |
| 22:C:1029:CLA:CMD  | 22:C:1031:CLA:CAB  | 2.68                     | 0.69              |
| 5:E:57:ALA:HB3     | 5:E:60:GLN:HG2     | 1.73                     | 0.69              |
| 7:H:17:GLU:HG3     | 7:H:20:LYS:HE2     | 1.73                     | 0.69              |
| 1:a:5344:ALA:HB1   | 3:c:5357:ARG:NH2   | 2.08                     | 0.69              |
| 22:b:6009:CLA:HAA2 | 25:h:6049:BCR:H363 | 1.74                     | 0.69              |
| 22:b:6012:CLA:HMB1 | 22:b:6015:CLA:CBB  | 2.20                     | 0.69              |
| 3:c:5166:ILE:HD12  | 3:c:5249:ILE:CD1   | 2.22                     | 0.69              |
| 3:c:5295:THR:HG22  | 3:c:5296:VAL:HG13  | 1.74                     | 0.69              |
| 1:A:124:SER:OG     | 1:A:151:LEU:HD11   | 1.92                     | 0.69              |
| 2:B:363:PHE:CD2    | 2:B:363:PHE:N      | 2.59                     | 0.69              |
| 2:B:475:PHE:CD1    | 4:D:140:PRO:CD     | 2.75                     | 0.69              |
| 22:B:1009:CLA:CBA  | 22:B:1009:CLA:CHA  | 2.70                     | 0.69              |
| 4:D:26:ARG:HG2     | 4:D:26:ARG:O       | 1.92                     | 0.69              |
| 13:O:76:PHE:HE2    | 13:O:132:VAL:HG21  | 1.56                     | 0.69              |
| 3:c:5327:ASN:HD22  | 3:c:5330:SER:H     | 1.41                     | 0.69              |
| 22:d:6005:CLA:CBC  | 22:d:6004:CLA:CBB  | 2.64                     | 0.69              |
| 15:u:5029:ASN:O    | 15:u:5097:ARG:NE   | 2.24                     | 0.69              |
| 15:u:5059:GLU:C    | 15:u:5061:VAL:H    | 1.98                     | 0.69              |
| 1:A:228:THR:HG22   | 1:A:229:GLU:N      | 2.07                     | 0.69              |
| 2:B:10:THR:O       | 2:B:13:ILE:HG22    | 1.91                     | 0.69              |
| 2:B:13:ILE:HG13    | 2:B:14:ASN:N       | 2.06                     | 0.69              |
| 2:B:144:PHE:HE1    | 2:B:210:ILE:HG23   | 1.55                     | 0.69              |
| 22:B:1018:CLA:H102 | 22:B:1023:CLA:CBA  | 2.23                     | 0.69              |
| 22:B:1019:CLA:HBC3 | 22:B:1019:CLA:HMC3 | 1.74                     | 0.69              |
| 3:C:327:ASN:HD22   | 3:C:330:SER:H      | 1.41                     | 0.69              |
| 3:C:438:LEU:O      | 3:C:438:LEU:HD13   | 1.92                     | 0.69              |
| 22:C:1025:CLA:HED3 | 22:C:1025:CLA:CAD  | 2.21                     | 0.69              |
| 4:D:57:SER:OG      | 4:D:65:SER:HB3     | 1.92                     | 0.69              |
| 4:D:101:PHE:O      | 4:D:105:CYS:HB2    | 1.92                     | 0.69              |
| 25:T:6046:BCR:C40  | 2:b:5036:SER:HB3   | 2.15                     | 0.69              |
| 1:a:5183:MET:SD    | 22:d:6005:CLA:HAC2 | 2.31                     | 0.69              |
| 24:a:6043:PQ9:H37  | 24:a:6043:PQ9:C28  | 2.22                     | 0.69              |
| 2:b:5030:VAL:HG12  | 22:b:6013:CLA:HHD  | 1.74                     | 0.69              |
| 22:b:6009:CLA:CBA  | 22:b:6009:CLA:CHA  | 2.70                     | 0.69              |
| 3:c:5450:ALA:CB    | 3:c:5456:GLU:HB3   | 2.22                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6025:CLA:C1   | 22:c:6025:CLA:H3A  | 2.22                     | 0.69              |
| 4:d:5057:SER:OG    | 4:d:5065:SER:HB3   | 1.92                     | 0.69              |
| 4:d:5091:LEU:HD23  | 4:d:5093:TRP:NE1   | 2.07                     | 0.69              |
| 24:d:6042:PQ9:C30  | 24:d:6042:PQ9:C34  | 2.67                     | 0.69              |
| 10:k:5032:PHE:CE1  | 25:k:6052:BCR:C23  | 2.75                     | 0.69              |
| 1:A:344:ALA:HB1    | 3:C:357:ARG:NH2    | 2.08                     | 0.69              |
| 4:D:91:LEU:HD23    | 4:D:93:TRP:NE1     | 2.07                     | 0.69              |
| 8:I:21:PHE:HD1     | 8:I:24:LEU:HD12    | 1.58                     | 0.69              |
| 10:K:24:VAL:CG2    | 18:Y:25:ILE:HG22   | 2.18                     | 0.69              |
| 16:V:38:LEU:HB2    | 16:V:45:ILE:CD1    | 2.23                     | 0.69              |
| 1:a:5212:CYS:O     | 4:d:5271:MET:HB3   | 1.92                     | 0.69              |
| 3:c:5049:LEU:HD11  | 22:c:6035:CLA:HMA1 | 1.73                     | 0.69              |
| 3:c:5342:MET:SD    | 3:c:5356:MET:HE2   | 2.32                     | 0.69              |
| 6:f:5022:ALA:O     | 6:f:5024:HIS:N     | 2.25                     | 0.69              |
| 8:i:5021:PHE:HD1   | 8:i:5024:LEU:HD12  | 1.58                     | 0.69              |
| 10:k:5032:PHE:HD1  | 25:k:6052:BCR:H383 | 1.55                     | 0.69              |
| 16:v:5151:ILE:HG12 | 16:v:5152:LEU:H    | 1.56                     | 0.69              |
| 1:A:140:ARG:CB     | 1:A:140:ARG:HH11   | 2.06                     | 0.69              |
| 1:A:183:MET:SD     | 22:D:1005:CLA:HAC2 | 2.31                     | 0.69              |
| 22:B:1021:CLA:H112 | 28:B:1060:MGE:H132 | 1.72                     | 0.69              |
| 3:C:100:GLY:HA2    | 3:C:196:VAL:CG1    | 2.23                     | 0.69              |
| 17:X:12:ILE:HA     | 17:X:16:LEU:HD22   | 1.74                     | 0.69              |
| 2:b:5040:TYR:C     | 2:b:5040:TYR:HD1   | 2.01                     | 0.69              |
| 22:b:6012:CLA:O1A  | 22:b:6020:CLA:H141 | 1.90                     | 0.69              |
| 28:b:6060:MGE:H211 | 28:b:6060:MGE:H263 | 1.75                     | 0.69              |
| 4:d:5126:MET:HE3   | 4:d:5146:PHE:HD2   | 1.57                     | 0.69              |
| 4:d:5198:MET:SD    | 22:d:6005:CLA:HED3 | 2.33                     | 0.69              |
| 28:d:6062:MGE:O6D  | 11:l:5015:THR:HG21 | 1.92                     | 0.69              |
| 1:A:244:GLU:HG3    | 4:D:242:GLU:HA     | 1.75                     | 0.69              |
| 22:A:1003:CLA:C4   | 23:A:1038:PHO:C3B  | 2.70                     | 0.69              |
| 3:C:453:ALA:HB2    | 8:I:31:ASN:HD22    | 1.57                     | 0.69              |
| 4:D:126:MET:HE3    | 4:D:146:PHE:HD2    | 1.57                     | 0.69              |
| 4:D:184:PHE:CE2    | 4:D:188:PHE:CD1    | 2.81                     | 0.69              |
| 1:a:5140:ARG:CB    | 1:a:5140:ARG:HH11  | 2.06                     | 0.69              |
| 22:b:6010:CLA:H172 | 29:b:6058:DGD:HA82 | 1.72                     | 0.69              |
| 22:c:6035:CLA:HBB1 | 22:c:6035:CLA:CHC  | 2.14                     | 0.69              |
| 4:d:5023:LYS:HE3   | 4:d:5135:LEU:HD11  | 1.75                     | 0.69              |
| 4:d:5169:PHE:CA    | 27:d:6068:IOD:I    | 3.11                     | 0.69              |
| 13:o:5215:ARG:HG2  | 13:o:5215:ARG:HH11 | 1.57                     | 0.69              |
| 24:A:1043:PQ9:C28  | 24:A:1043:PQ9:H37  | 2.22                     | 0.69              |
| 2:B:30:VAL:HG12    | 22:B:1013:CLA:HHD  | 1.74                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:45:LEU:HD13    | 3:C:139:THR:OG1    | 1.93                     | 0.69              |
| 3:C:167:VAL:HG12   | 3:C:168:LEU:CD1    | 2.20                     | 0.69              |
| 4:D:198:MET:SD     | 22:D:1005:CLA:HED3 | 2.33                     | 0.69              |
| 9:J:21:VAL:O       | 9:J:25:VAL:HB      | 1.92                     | 0.69              |
| 9:J:25:VAL:HA      | 9:J:28:PHE:HD2     | 1.58                     | 0.69              |
| 25:K:1051:BCR:C8   | 25:K:1051:BCR:H321 | 2.23                     | 0.69              |
| 15:U:45:LEU:HD21   | 15:U:75:LEU:HD12   | 1.73                     | 0.69              |
| 16:V:50:LYS:HE2    | 16:V:50:LYS:HA     | 1.73                     | 0.69              |
| 18:Y:45:ASN:HD22   | 18:Y:45:ASN:C      | 2.00                     | 0.69              |
| 1:a:5254:TYR:CD1   | 1:a:5255:PHE:N     | 2.61                     | 0.69              |
| 3:c:5453:ALA:HB2   | 8:i:5031:ASN:HD22  | 1.57                     | 0.69              |
| 22:c:6030:CLA:H121 | 22:c:6030:CLA:H171 | 1.72                     | 0.69              |
| 4:d:5210:LEU:CD2   | 4:d:5274:VAL:HG21  | 2.23                     | 0.69              |
| 7:h:5014:LEU:HD12  | 7:h:5014:LEU:H     | 1.57                     | 0.69              |
| 13:o:5101:THR:O    | 13:o:5130:GLN:HG3  | 1.93                     | 0.69              |
| 16:v:5038:LEU:HB2  | 16:v:5045:ILE:CD1  | 2.23                     | 0.69              |
| 16:v:5066:CYS:SG   | 31:v:6041:HEM:HAC  | 2.33                     | 0.69              |
| 1:A:272:HIS:CB     | 4:D:218:VAL:HG11   | 2.23                     | 0.69              |
| 2:B:69:LEU:HD11    | 22:B:1011:CLA:OBD  | 1.93                     | 0.69              |
| 2:B:152:GLY:O      | 2:B:156:PHE:HB2    | 1.91                     | 0.69              |
| 2:B:284:ILE:HG23   | 2:B:305:ILE:HD13   | 1.73                     | 0.69              |
| 2:B:475:PHE:N      | 2:B:475:PHE:HD2    | 1.90                     | 0.69              |
| 22:B:1011:CLA:HMD3 | 22:B:1014:CLA:HMB2 | 1.74                     | 0.69              |
| 22:B:1021:CLA:HMA3 | 22:B:1021:CLA:C2   | 2.23                     | 0.69              |
| 3:C:81:MET:HG3     | 3:C:86:LEU:HD13    | 1.73                     | 0.69              |
| 3:C:417:VAL:CG1    | 16:V:68:VAL:CB     | 2.70                     | 0.69              |
| 22:C:1035:CLA:HBB1 | 22:C:1035:CLA:CHC  | 2.14                     | 0.69              |
| 4:D:185:PHE:CD1    | 22:D:1004:CLA:HMD2 | 2.28                     | 0.69              |
| 4:D:265:ARG:HH11   | 4:D:265:ARG:CG     | 2.03                     | 0.69              |
| 22:D:1008:CLA:HBB1 | 22:D:1008:CLA:CHC  | 2.13                     | 0.69              |
| 8:I:24:LEU:C       | 8:I:26:GLY:H       | 2.01                     | 0.69              |
| 16:V:66:CYS:SG     | 31:V:1041:HEM:HAC  | 2.33                     | 0.69              |
| 16:V:151:ILE:HG12  | 16:V:152:LEU:H     | 1.56                     | 0.69              |
| 22:b:6011:CLA:HMD3 | 22:b:6014:CLA:HMB2 | 1.74                     | 0.69              |
| 22:b:6018:CLA:H102 | 22:b:6023:CLA:CBA  | 2.23                     | 0.69              |
| 3:c:5275:SER:HB3   | 22:c:6033:CLA:HED3 | 1.71                     | 0.69              |
| 4:d:5221:THR:HG23  | 4:d:5248:THR:HB    | 1.75                     | 0.69              |
| 4:d:5265:ARG:HG3   | 4:d:5265:ARG:NH1   | 2.04                     | 0.69              |
| 16:v:5050:LYS:HE2  | 16:v:5050:LYS:HA   | 1.73                     | 0.69              |
| 22:B:1012:CLA:HMB1 | 22:B:1015:CLA:CBB  | 2.20                     | 0.69              |
| 22:B:1013:CLA:HAB  | 22:B:1014:CLA:H52  | 1.72                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:91:HIS:NE2     | 22:C:1026:CLA:HED1 | 2.07                     | 0.69              |
| 22:C:1032:CLA:O2D  | 22:C:1032:CLA:H2A  | 1.92                     | 0.69              |
| 29:C:1057:DGD:HAS2 | 28:D:1059:MGE:H232 | 1.74                     | 0.69              |
| 4:D:210:LEU:CD2    | 4:D:274:VAL:HG21   | 2.23                     | 0.69              |
| 11:L:4:ASN:OD1     | 11:L:5:PRO:HD2     | 1.93                     | 0.69              |
| 2:b:5069:LEU:HD11  | 22:b:6011:CLA:OBD  | 1.93                     | 0.69              |
| 2:b:5119:ASP:OD2   | 7:h:5002:ALA:HA    | 1.93                     | 0.69              |
| 2:b:5363:PHE:HD2   | 2:b:5363:PHE:N     | 1.91                     | 0.69              |
| 3:c:5056:HIS:HA    | 3:c:5059:LEU:CD1   | 2.23                     | 0.69              |
| 3:c:5417:VAL:CG1   | 16:v:5068:VAL:CB   | 2.70                     | 0.69              |
| 4:d:5329:MET:C     | 4:d:5331:PRO:HD2   | 2.17                     | 0.69              |
| 22:d:6008:CLA:C19  | 22:d:6008:CLA:H141 | 2.18                     | 0.69              |
| 25:h:6049:BCR:HC8  | 25:h:6049:BCR:H321 | 1.75                     | 0.69              |
| 10:k:5028:ILE:O    | 10:k:5029:PRO:C    | 2.36                     | 0.69              |
| 2:B:13:ILE:HD12    | 2:B:234:ILE:CG2    | 2.23                     | 0.68              |
| 3:C:457:LYS:NZ     | 4:D:228:GLY:HA2    | 2.08                     | 0.68              |
| 22:C:1035:CLA:C8   | 25:C:1052:BCR:H403 | 2.10                     | 0.68              |
| 4:D:207:GLY:CA     | 4:D:274:VAL:HG11   | 2.23                     | 0.68              |
| 22:K:1034:CLA:CGD  | 22:K:1034:CLA:CAA  | 2.65                     | 0.68              |
| 16:V:64:ALA:HB1    | 16:V:68:VAL:HA     | 1.74                     | 0.68              |
| 16:V:66:CYS:O      | 16:V:73:LYS:HG3    | 1.93                     | 0.68              |
| 2:b:5249:ALA:HB1   | 2:b:5459:ALA:HB2   | 1.73                     | 0.68              |
| 3:c:5199:ILE:H     | 3:c:5199:ILE:HD12  | 1.58                     | 0.68              |
| 3:c:5278:ALA:O     | 3:c:5282:MET:HE2   | 1.93                     | 0.68              |
| 4:d:5109:GLY:O     | 4:d:5111:TRP:N     | 2.27                     | 0.68              |
| 4:d:5185:PHE:CD1   | 22:d:6004:CLA:HMD2 | 2.28                     | 0.68              |
| 9:j:5021:VAL:O     | 9:j:5025:VAL:HB    | 1.92                     | 0.68              |
| 9:j:5025:VAL:HA    | 9:j:5028:PHE:HD2   | 1.58                     | 0.68              |
| 1:A:254:TYR:CD1    | 1:A:255:PHE:N      | 2.61                     | 0.68              |
| 2:B:277:SER:O      | 2:B:279:TYR:N      | 2.23                     | 0.68              |
| 22:C:1030:CLA:CAD  | 22:C:1030:CLA:CED  | 2.71                     | 0.68              |
| 4:D:92:LEU:O       | 4:D:99:GLY:N       | 2.26                     | 0.68              |
| 5:E:34:GLY:HA2     | 6:F:32:PHE:HE1     | 1.56                     | 0.68              |
| 1:a:5210:LEU:HA    | 23:d:6039:PHO:HAC2 | 1.75                     | 0.68              |
| 22:a:6003:CLA:C4   | 23:a:6038:PHO:C3B  | 2.70                     | 0.68              |
| 2:b:5249:ALA:HB2   | 22:b:6012:CLA:HBC1 | 1.73                     | 0.68              |
| 22:b:6011:CLA:C2   | 22:b:6013:CLA:H92  | 2.22                     | 0.68              |
| 22:c:6029:CLA:H43  | 25:c:6054:BCR:C32  | 2.22                     | 0.68              |
| 23:d:6039:PHO:HHD  | 23:d:6039:PHO:CBC  | 2.23                     | 0.68              |
| 25:k:6051:BCR:H321 | 25:k:6051:BCR:C8   | 2.23                     | 0.68              |
| 22:A:1003:CLA:H203 | 22:D:1005:CLA:H92  | 1.75                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:363:PHE:N      | 2:B:363:PHE:HD2    | 1.91                     | 0.68              |
| 22:B:1023:CLA:HMC3 | 22:B:1023:CLA:HBC2 | 1.73                     | 0.68              |
| 25:B:1045:BCR:C8   | 25:B:1045:BCR:C33  | 2.66                     | 0.68              |
| 28:B:1060:MGE:H211 | 28:B:1060:MGE:H263 | 1.75                     | 0.68              |
| 4:D:23:LYS:HE3     | 4:D:135:LEU:HD11   | 1.75                     | 0.68              |
| 4:D:221:THR:O      | 4:D:244:TYR:HA     | 1.93                     | 0.68              |
| 22:D:1008:CLA:HMC3 | 22:D:1008:CLA:CBC  | 2.23                     | 0.68              |
| 1:a:5039:PRO:HD2   | 22:a:6007:CLA:HBB2 | 1.74                     | 0.68              |
| 26:a:6063:LHG:H321 | 22:k:6034:CLA:C15  | 2.21                     | 0.68              |
| 2:b:5025:MET:HG3   | 25:b:6045:BCR:H391 | 1.74                     | 0.68              |
| 3:c:5049:LEU:HD21  | 22:c:6035:CLA:CMA  | 2.15                     | 0.68              |
| 3:c:5081:MET:HG3   | 3:c:5086:LEU:HD13  | 1.73                     | 0.68              |
| 3:c:5091:HIS:NE2   | 22:c:6026:CLA:HED1 | 2.07                     | 0.68              |
| 3:c:5348:GLU:CD    | 3:c:5373:ASN:HB3   | 2.19                     | 0.68              |
| 22:c:6032:CLA:H2A  | 22:c:6032:CLA:O2D  | 1.92                     | 0.68              |
| 4:d:5045:LEU:HG    | 4:d:5049:LEU:CD1   | 2.24                     | 0.68              |
| 22:k:6034:CLA:O2A  | 22:k:6034:CLA:CHA  | 2.41                     | 0.68              |
| 25:k:6052:BCR:H312 | 20:z:5009:LEU:HD11 | 1.75                     | 0.68              |
| 11:l:5008:GLN:H    | 11:l:5008:GLN:HE21 | 1.41                     | 0.68              |
| 15:u:5045:LEU:HD11 | 15:u:5075:LEU:HD11 | 1.75                     | 0.68              |
| 22:A:1006:CLA:C16  | 24:A:1043:PQ9:H443 | 2.22                     | 0.68              |
| 2:B:36:SER:HB3     | 25:t:1046:BCR:C40  | 2.15                     | 0.68              |
| 2:B:394:GLN:HB3    | 15:U:17:LEU:CD2    | 2.23                     | 0.68              |
| 22:B:1009:CLA:HBB1 | 22:B:1009:CLA:CHC  | 2.15                     | 0.68              |
| 25:B:1047:BCR:H14C | 25:t:1046:BCR:C39  | 2.24                     | 0.68              |
| 3:C:88:LEU:HD11    | 22:C:1027:CLA:HBC2 | 1.74                     | 0.68              |
| 10:K:43:VAL:O      | 10:K:43:VAL:HG12   | 1.94                     | 0.68              |
| 15:U:45:LEU:HD11   | 15:U:75:LEU:HD11   | 1.75                     | 0.68              |
| 1:a:5269:ARG:HD3   | 4:d:5222:LEU:CD1   | 2.20                     | 0.68              |
| 2:b:5327:THR:HG21  | 12:m:5004:ASN:ND2  | 2.09                     | 0.68              |
| 3:c:5334:PRO:HA    | 13:o:5179:THR:CB   | 2.23                     | 0.68              |
| 29:c:6056:DGD:HBG2 | 29:c:6056:DGD:HBF2 | 0.81                     | 0.68              |
| 4:d:5092:LEU:O     | 4:d:5099:GLY:N     | 2.26                     | 0.68              |
| 5:e:5075:GLN:O     | 5:e:5076:VAL:C     | 2.36                     | 0.68              |
| 1:A:279:ARG:CZ     | 1:A:283:VAL:CG2    | 2.71                     | 0.68              |
| 2:B:10:THR:O       | 2:B:11:VAL:C       | 2.36                     | 0.68              |
| 2:B:25:MET:HG3     | 25:B:1045:BCR:H391 | 1.74                     | 0.68              |
| 25:B:1047:BCR:H331 | 25:B:1047:BCR:C8   | 2.14                     | 0.68              |
| 3:C:117:VAL:HA     | 25:Z:1053:BCR:H343 | 1.76                     | 0.68              |
| 4:D:59:TYR:O       | 5:E:66:VAL:HG23    | 1.94                     | 0.68              |
| 4:D:109:GLY:O      | 4:D:111:TRP:N      | 2.27                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:L:14:ARG:CA     | 12:M:26:TYR:HE1    | 2.05                     | 0.68              |
| 22:b:6011:CLA:O1A  | 22:b:6011:CLA:C3A  | 2.30                     | 0.68              |
| 3:c:5089:ILE:HG23  | 3:c:5111:PHE:CE2   | 2.28                     | 0.68              |
| 3:c:5167:VAL:HG12  | 3:c:5168:LEU:CD1   | 2.20                     | 0.68              |
| 22:c:6031:CLA:CB   | 22:c:6031:CLA:CHD  | 2.71                     | 0.68              |
| 5:e:5037:PHE:HE1   | 5:e:5046:VAL:HG21  | 1.57                     | 0.68              |
| 5:e:5079:PHE:O     | 5:e:5083:LEU:HD13  | 1.94                     | 0.68              |
| 12:m:5009:ILE:HD12 | 12:m:5009:ILE:H    | 1.58                     | 0.68              |
| 18:y:5021:GLN:O    | 18:y:5025:ILE:HG23 | 1.94                     | 0.68              |
| 2:B:40:TYR:C       | 2:B:40:TYR:HD1     | 2.01                     | 0.68              |
| 2:B:119:ASP:OD2    | 7:H:2:ALA:HA       | 1.94                     | 0.68              |
| 2:B:327:THR:HG21   | 12:M:4:ASN:ND2     | 2.09                     | 0.68              |
| 3:C:49:LEU:HB3     | 3:C:133:ALA:CA     | 2.18                     | 0.68              |
| 4:D:254:SER:OG     | 4:D:260:ALA:HB2    | 1.93                     | 0.68              |
| 13:O:101:THR:O     | 13:O:130:GLN:HG3   | 1.93                     | 0.68              |
| 13:O:190:LEU:C     | 13:O:190:LEU:CD2   | 2.67                     | 0.68              |
| 1:a:5256:GLY:C     | 1:a:5261:GLN:HA    | 2.18                     | 0.68              |
| 2:b:5323:GLY:HA3   | 2:b:5326:ARG:HG3   | 1.74                     | 0.68              |
| 3:c:5045:LEU:HD13  | 3:c:5139:THR:OG1   | 1.93                     | 0.68              |
| 3:c:5199:ILE:HG12  | 3:c:5234:VAL:HG11  | 1.76                     | 0.68              |
| 4:d:5184:PHE:CE2   | 4:d:5188:PHE:CD1   | 2.81                     | 0.68              |
| 7:h:5011:LEU:C     | 7:h:5013:PRO:HD2   | 2.19                     | 0.68              |
| 14:t:5012:CYS:CB   | 27:t:6066:IOD:I    | 3.07                     | 0.68              |
| 17:x:5012:ILE:HA   | 17:x:5016:LEU:HD22 | 1.74                     | 0.68              |
| 1:A:47:CYS:SG      | 25:A:1044:BCR:H373 | 2.34                     | 0.68              |
| 1:A:196:PRO:HG3    | 3:C:404:LEU:CD1    | 2.23                     | 0.68              |
| 1:A:330:VAL:CG1    | 4:D:348:ARG:HA     | 2.24                     | 0.68              |
| 2:B:32:GLY:HA3     | 25:B:1047:BCR:C36  | 2.24                     | 0.68              |
| 4:D:15:PHE:CE1     | 4:D:32:TRP:HZ2     | 2.12                     | 0.68              |
| 4:D:352:LEU:HD23   | 4:D:352:LEU:H      | 1.59                     | 0.68              |
| 7:H:13:PRO:HG2     | 7:H:14:LEU:H       | 1.59                     | 0.68              |
| 1:a:5047:CYS:SG    | 25:a:6044:BCR:H373 | 2.34                     | 0.68              |
| 1:a:5062:GLY:HA2   | 1:a:5087:ASN:HB2   | 1.76                     | 0.68              |
| 2:b:5363:PHE:N     | 2:b:5363:PHE:CD2   | 2.59                     | 0.68              |
| 22:b:6019:CLA:C19  | 22:b:6021:CLA:C7   | 2.71                     | 0.68              |
| 4:d:5188:PHE:CD2   | 4:d:5326:ARG:HG2   | 2.29                     | 0.68              |
| 13:o:5082:PRO:CG   | 13:o:5089:ALA:CB   | 2.71                     | 0.68              |
| 13:o:5196:SER:OG   | 13:o:5197:ALA:N    | 2.26                     | 0.68              |
| 2:B:105:GLY:CA     | 25:B:1047:BCR:H402 | 2.19                     | 0.68              |
| 22:B:1009:CLA:HAA2 | 25:H:1049:BCR:H363 | 1.74                     | 0.68              |
| 22:B:1019:CLA:H193 | 22:B:1021:CLA:C7   | 2.24                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:295:THR:HG22   | 3:C:296:VAL:HG13   | 1.74                     | 0.68              |
| 4:D:267:LEU:HD22   | 4:D:268:HIS:CE1    | 2.28                     | 0.68              |
| 2:b:5010:THR:O     | 2:b:5011:VAL:C     | 2.37                     | 0.68              |
| 22:b:6019:CLA:H193 | 22:b:6021:CLA:C7   | 2.24                     | 0.68              |
| 22:b:6019:CLA:HBC3 | 22:b:6019:CLA:HMC3 | 1.74                     | 0.68              |
| 3:c:5117:VAL:HA    | 25:z:6053:BCR:H343 | 1.76                     | 0.68              |
| 3:c:5420:VAL:HB    | 3:c:5425:TRP:NE1   | 2.09                     | 0.68              |
| 3:c:5451:ALA:HA    | 3:c:5456:GLU:HG2   | 1.75                     | 0.68              |
| 4:d:5043:LEU:HD23  | 4:d:5043:LEU:N     | 2.08                     | 0.68              |
| 4:d:5050:THR:CG2   | 25:d:6050:BCR:H333 | 2.23                     | 0.68              |
| 22:d:6008:CLA:HMC3 | 22:d:6008:CLA:CBC  | 2.23                     | 0.68              |
| 25:d:6050:BCR:C21  | 28:d:6059:MGE:C3A  | 2.72                     | 0.68              |
| 10:k:5043:VAL:HG12 | 10:k:5043:VAL:O    | 1.94                     | 0.68              |
| 1:A:256:GLY:C      | 1:A:261:GLN:HA     | 2.18                     | 0.68              |
| 22:B:1019:CLA:C19  | 22:B:1021:CLA:C7   | 2.71                     | 0.68              |
| 3:C:89:ILE:HG23    | 3:C:111:PHE:CE2    | 2.28                     | 0.68              |
| 3:C:318:LEU:HD21   | 3:C:328:VAL:HG11   | 1.75                     | 0.68              |
| 4:D:43:LEU:N       | 4:D:43:LEU:HD23    | 2.08                     | 0.68              |
| 4:D:171:PRO:HA     | 4:D:181:PHE:CD2    | 2.28                     | 0.68              |
| 12:M:34:LYS:HD2    | 12:m:5032:GLN:CD   | 2.19                     | 0.68              |
| 13:O:82:PRO:CG     | 13:O:89:ALA:CB     | 2.71                     | 0.68              |
| 18:Y:21:GLN:O      | 18:Y:25:ILE:HG23   | 1.94                     | 0.68              |
| 1:a:5228:THR:HG22  | 1:a:5229:GLU:N     | 2.07                     | 0.68              |
| 22:c:6030:CLA:CAD  | 22:c:6030:CLA:CED  | 2.71                     | 0.68              |
| 29:c:6057:DGD:HAS2 | 28:d:6059:MGE:H232 | 1.74                     | 0.68              |
| 4:d:5015:PHE:CE1   | 4:d:5032:TRP:HZ2   | 2.12                     | 0.68              |
| 4:d:5101:PHE:O     | 4:d:5105:CYS:HB2   | 1.92                     | 0.68              |
| 1:A:78:ILE:HD12    | 1:A:78:ILE:N       | 2.09                     | 0.68              |
| 1:A:149:ALA:HB1    | 1:A:283:VAL:CG1    | 2.24                     | 0.68              |
| 2:B:12:LEU:O       | 2:B:13:ILE:HG23    | 1.94                     | 0.68              |
| 3:C:56:HIS:HA      | 3:C:59:LEU:CD1     | 2.23                     | 0.68              |
| 3:C:451:ALA:HA     | 3:C:456:GLU:HG2    | 1.75                     | 0.68              |
| 22:C:1030:CLA:HMB2 | 22:C:1031:CLA:C4B  | 2.07                     | 0.68              |
| 25:C:1052:BCR:H312 | 20:Z:9:LEU:HD11    | 1.75                     | 0.68              |
| 4:D:218:VAL:HG12   | 4:D:219:GLU:N      | 2.08                     | 0.68              |
| 7:H:11:LEU:C       | 7:H:13:PRO:HD2     | 2.19                     | 0.68              |
| 13:O:82:PRO:HG2    | 13:O:89:ALA:CB     | 2.24                     | 0.68              |
| 16:V:101:TYR:HE1   | 16:V:118:HIS:HD1   | 1.42                     | 0.68              |
| 16:V:103:LYS:HD2   | 16:V:121:LEU:HD13  | 1.75                     | 0.68              |
| 1:a:5224:ILE:HD13  | 1:a:5225:ARG:H     | 1.59                     | 0.68              |
| 2:b:5032:GLY:HA3   | 25:b:6047:BCR:C36  | 2.24                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5266:TRP:HB3   | 3:c:5271:TYR:OH    | 1.94                     | 0.68              |
| 4:d:5059:TYR:O     | 5:e:5066:VAL:HG23  | 1.94                     | 0.68              |
| 4:d:5095:PRO:CG    | 17:x:5015:SER:HB2  | 2.23                     | 0.68              |
| 4:d:5207:GLY:CA    | 4:d:5274:VAL:HG11  | 2.23                     | 0.68              |
| 4:d:5218:VAL:HG12  | 4:d:5219:GLU:N     | 2.09                     | 0.68              |
| 13:o:5242:GLU:CD   | 13:o:5260:LYS:HD3  | 2.19                     | 0.68              |
| 25:z:6053:BCR:C38  | 25:z:6053:BCR:C23  | 2.59                     | 0.68              |
| 1:A:337:HIS:O      | 4:D:351:ALA:CB     | 2.36                     | 0.67              |
| 3:C:278:ALA:O      | 3:C:282:MET:HE2    | 1.94                     | 0.67              |
| 3:C:343:ARG:HG2    | 3:C:348:GLU:O      | 1.94                     | 0.67              |
| 3:C:417:VAL:HG12   | 16:V:68:VAL:CB     | 2.21                     | 0.67              |
| 4:D:61:HIS:CE1     | 4:D:80:THR:HG23    | 2.30                     | 0.67              |
| 25:H:1049:BCR:HC8  | 25:H:1049:BCR:H321 | 1.76                     | 0.67              |
| 12:M:35:SER:O      | 12:M:36:SER:HB2    | 1.94                     | 0.67              |
| 15:U:29:ASN:O      | 15:U:97:ARG:NE     | 2.24                     | 0.67              |
| 1:a:5094:TYR:CE1   | 1:a:5105:TRP:HA    | 2.29                     | 0.67              |
| 2:b:5451:PHE:CZ    | 22:b:6012:CLA:O1D  | 2.47                     | 0.67              |
| 3:c:5046:SER:CB    | 3:c:5141:GLU:CB    | 2.59                     | 0.67              |
| 5:e:5020:TRP:O     | 5:e:5024:SER:HB3   | 1.94                     | 0.67              |
| 12:m:5035:SER:O    | 12:m:5036:SER:HB2  | 1.94                     | 0.67              |
| 13:o:5190:LEU:C    | 13:o:5190:LEU:CD2  | 2.67                     | 0.67              |
| 15:u:5025:ILE:HG21 | 15:u:5035:PHE:HE2  | 1.59                     | 0.67              |
| 16:v:5101:TYR:HE1  | 16:v:5118:HIS:HD1  | 1.43                     | 0.67              |
| 1:A:174:LEU:HD22   | 23:A:1038:PHO:H152 | 1.76                     | 0.67              |
| 22:A:1007:CLA:CHA  | 22:A:1007:CLA:CBA  | 2.72                     | 0.67              |
| 22:B:1012:CLA:CAB  | 22:B:1015:CLA:HBB2 | 2.24                     | 0.67              |
| 22:K:1034:CLA:O2A  | 22:K:1034:CLA:CHA  | 2.41                     | 0.67              |
| 16:V:54:GLU:O      | 16:V:58:LEU:HD23   | 1.94                     | 0.67              |
| 22:a:6003:CLA:H203 | 22:d:6005:CLA:H92  | 1.75                     | 0.67              |
| 22:b:6023:CLA:O1D  | 22:b:6023:CLA:H2A  | 1.95                     | 0.67              |
| 29:b:6058:DGD:O2D  | 29:b:6058:DGD:HG31 | 1.95                     | 0.67              |
| 3:c:5117:VAL:HG12  | 3:c:5118:HIS:H     | 1.56                     | 0.67              |
| 4:d:5021:TRP:O     | 4:d:5026:ARG:NH2   | 2.28                     | 0.67              |
| 4:d:5274:VAL:HG22  | 24:d:6042:PQ9:H293 | 1.76                     | 0.67              |
| 8:i:5024:LEU:C     | 8:i:5026:GLY:H     | 2.01                     | 0.67              |
| 15:u:5059:GLU:O    | 15:u:5061:VAL:N    | 2.27                     | 0.67              |
| 1:A:212:CYS:SG     | 4:D:210:LEU:HB3    | 2.34                     | 0.67              |
| 1:A:224:ILE:HG23   | 1:A:225:ARG:N      | 2.08                     | 0.67              |
| 2:B:221:PRO:O      | 7:H:21:VAL:HG23    | 1.94                     | 0.67              |
| 2:B:271:THR:HG22   | 2:B:274:GLN:NE2    | 2.10                     | 0.67              |
| 2:B:429:ILE:HD12   | 2:B:429:ILE:N      | 2.10                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1023:CLA:O1D  | 22:B:1023:CLA:H2A  | 1.95                     | 0.67              |
| 22:C:1029:CLA:HMC1 | 22:C:1029:CLA:CBC  | 2.25                     | 0.67              |
| 25:D:1050:BCR:C21  | 28:D:1059:MGE:C3A  | 2.72                     | 0.67              |
| 1:a:5078:ILE:N     | 1:a:5078:ILE:HD12  | 2.09                     | 0.67              |
| 1:a:5244:GLU:HG3   | 4:d:5242:GLU:HA    | 1.75                     | 0.67              |
| 1:a:5247:ASN:HD21  | 2:b:5486:LEU:HB3   | 1.59                     | 0.67              |
| 2:b:5221:PRO:O     | 7:h:5021:VAL:HG23  | 1.94                     | 0.67              |
| 3:c:5457:LYS:NZ    | 4:d:5228:GLY:HA2   | 2.07                     | 0.67              |
| 22:c:6029:CLA:HMC1 | 22:c:6029:CLA:CBC  | 2.25                     | 0.67              |
| 4:d:5126:MET:HE2   | 4:d:5143:ALA:O     | 1.94                     | 0.67              |
| 4:d:5221:THR:O     | 4:d:5244:TYR:HA    | 1.93                     | 0.67              |
| 4:d:5352:LEU:H     | 4:d:5352:LEU:HD23  | 1.59                     | 0.67              |
| 8:i:5012:VAL:O     | 8:i:5016:VAL:HG23  | 1.95                     | 0.67              |
| 8:i:5014:PHE:C     | 8:i:5014:PHE:CD1   | 2.67                     | 0.67              |
| 14:t:5018:PHE:HD1  | 25:t:1046:BCR:C33  | 2.08                     | 0.67              |
| 2:B:433:ASP:C      | 2:B:433:ASP:OD1    | 2.37                     | 0.67              |
| 3:C:199:ILE:HG12   | 3:C:234:VAL:HG11   | 1.76                     | 0.67              |
| 4:D:45:LEU:HG      | 4:D:49:LEU:HD12    | 1.75                     | 0.67              |
| 4:D:95:PRO:CG      | 17:X:15:SER:HB2    | 2.23                     | 0.67              |
| 24:D:1042:PQ9:H301 | 24:D:1042:PQ9:C34  | 2.06                     | 0.67              |
| 5:E:8:ARG:HE       | 6:F:13:TYR:CB      | 2.02                     | 0.67              |
| 25:T:6046:BCR:H323 | 25:T:6046:BCR:HC41 | 1.77                     | 0.67              |
| 15:U:59:GLU:O      | 15:U:61:VAL:N      | 2.27                     | 0.67              |
| 7:h:5013:PRO:HG2   | 7:h:5014:LEU:H     | 1.59                     | 0.67              |
| 16:v:5066:CYS:O    | 16:v:5073:LYS:HG3  | 1.93                     | 0.67              |
| 2:B:31:ALA:HB2     | 22:B:1013:CLA:HAC1 | 1.74                     | 0.67              |
| 22:B:1019:CLA:HBA2 | 22:B:1019:CLA:HBD  | 1.76                     | 0.67              |
| 3:C:42:LEU:CD1     | 3:C:48:LYS:HG2     | 2.24                     | 0.67              |
| 4:D:110:LEU:O      | 4:D:114:ILE:HG13   | 1.95                     | 0.67              |
| 4:D:250:ASN:HB2    | 4:D:260:ALA:CB     | 2.20                     | 0.67              |
| 23:D:1039:PHO:H42  | 23:D:1039:PHO:O2A  | 1.95                     | 0.67              |
| 13:O:141:ARG:HH11  | 13:O:141:ARG:CG    | 2.07                     | 0.67              |
| 13:O:242:GLU:CD    | 13:O:260:LYS:HD3   | 2.19                     | 0.67              |
| 25:T:6046:BCR:C39  | 25:b:6047:BCR:H14C | 2.24                     | 0.67              |
| 16:V:35:THR:HA     | 16:V:46:THR:HA     | 1.77                     | 0.67              |
| 1:a:5330:VAL:CG1   | 4:d:5348:ARG:HA    | 2.24                     | 0.67              |
| 2:b:5220:ARG:CD    | 2:b:5221:PRO:HD2   | 2.20                     | 0.67              |
| 2:b:5394:GLN:HB3   | 15:u:5017:LEU:CD2  | 2.23                     | 0.67              |
| 2:b:5429:ILE:HD12  | 2:b:5429:ILE:N     | 2.10                     | 0.67              |
| 4:d:5026:ARG:O     | 4:d:5026:ARG:HG2   | 1.92                     | 0.67              |
| 4:d:5198:MET:SD    | 22:d:6005:CLA:CED  | 2.83                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:e:5079:PHE:O     | 5:e:5083:LEU:HB2   | 1.95                     | 0.67              |
| 11:l:5030:LEU:HD23 | 11:l:5030:LEU:C    | 2.19                     | 0.67              |
| 1:A:224:ILE:HD13   | 1:A:225:ARG:H      | 1.59                     | 0.67              |
| 2:B:25:MET:HG3     | 25:B:1045:BCR:C40  | 2.25                     | 0.67              |
| 3:C:49:LEU:CD1     | 3:C:49:LEU:N       | 2.51                     | 0.67              |
| 3:C:348:GLU:CD     | 3:C:373:ASN:HB3    | 2.19                     | 0.67              |
| 22:C:1025:CLA:H2A  | 22:C:1025:CLA:O1D  | 1.94                     | 0.67              |
| 4:D:21:TRP:O       | 4:D:26:ARG:NH2     | 2.27                     | 0.67              |
| 4:D:45:LEU:HG      | 4:D:49:LEU:CD1     | 2.24                     | 0.67              |
| 4:D:188:PHE:CD2    | 4:D:326:ARG:HG2    | 2.29                     | 0.67              |
| 22:D:1004:CLA:HBB1 | 22:D:1004:CLA:CHC  | 2.15                     | 0.67              |
| 11:L:21:LEU:CB     | 14:T:16:LEU:HD21   | 2.24                     | 0.67              |
| 20:Z:43:GLY:O      | 20:Z:47:TRP:N      | 2.27                     | 0.67              |
| 2:b:5013:ILE:HD12  | 2:b:5234:ILE:CG2   | 2.23                     | 0.67              |
| 22:b:6019:CLA:HBD  | 22:b:6019:CLA:HBA2 | 1.76                     | 0.67              |
| 22:c:6025:CLA:O1D  | 22:c:6025:CLA:H2A  | 1.94                     | 0.67              |
| 4:d:5061:HIS:CE1   | 4:d:5080:THR:HG23  | 2.30                     | 0.67              |
| 13:o:5172:PHE:HB2  | 13:o:5221:GLY:N    | 2.08                     | 0.67              |
| 13:o:5202:GLN:OE1  | 13:o:5202:GLN:HA   | 1.93                     | 0.67              |
| 15:u:5046:ALA:HA   | 15:u:5049:ILE:HD12 | 1.77                     | 0.67              |
| 3:C:59:LEU:HD22    | 22:K:1034:CLA:HBD  | 1.77                     | 0.67              |
| 3:C:261:ARG:HA     | 3:C:266:TRP:CZ2    | 2.30                     | 0.67              |
| 3:C:334:PRO:HA     | 13:O:179:THR:CB    | 2.23                     | 0.67              |
| 4:D:221:THR:HG23   | 4:D:248:THR:HB     | 1.75                     | 0.67              |
| 5:E:79:PHE:O       | 5:E:83:LEU:HD13    | 1.94                     | 0.67              |
| 1:a:5109:GLY:C     | 1:a:5111:PRO:HD2   | 2.20                     | 0.67              |
| 1:a:5174:LEU:HD22  | 23:a:6038:PHO:H152 | 1.77                     | 0.67              |
| 22:b:6022:CLA:H11  | 22:b:6022:CLA:CHA  | 2.25                     | 0.67              |
| 3:c:5187:ASP:HB2   | 3:c:5230:LEU:CD1   | 2.25                     | 0.67              |
| 4:d:5254:SER:OG    | 4:d:5260:ALA:HB2   | 1.93                     | 0.67              |
| 1:A:94:TYR:CE1     | 1:A:105:TRP:HA     | 2.29                     | 0.67              |
| 1:A:109:GLY:C      | 1:A:111:PRO:HD2    | 2.20                     | 0.67              |
| 22:B:1019:CLA:H2A  | 22:B:1019:CLA:O1D  | 1.95                     | 0.67              |
| 4:D:50:THR:CG2     | 25:D:1050:BCR:H333 | 2.24                     | 0.67              |
| 23:D:1039:PHO:HHD  | 23:D:1039:PHO:CBC  | 2.23                     | 0.67              |
| 24:D:1042:PQ9:C30  | 24:D:1042:PQ9:C34  | 2.67                     | 0.67              |
| 25:K:1051:BCR:C23  | 25:K:1051:BCR:C40  | 2.64                     | 0.67              |
| 11:L:30:LEU:HD23   | 11:L:30:LEU:C      | 2.19                     | 0.67              |
| 1:a:5060:ILE:HG22  | 1:a:5061:ASP:N     | 2.10                     | 0.67              |
| 1:a:5279:ARG:HD2   | 4:d:5208:ALA:HB1   | 1.75                     | 0.67              |
| 3:c:5049:LEU:HD23  | 3:c:5052:ALA:N     | 2.08                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5171:PRO:HA    | 4:d:5181:PHE:CD2   | 2.29                     | 0.67              |
| 10:k:5035:LEU:O    | 10:k:5038:VAL:HG23 | 1.94                     | 0.67              |
| 11:l:5004:ASN:OD1  | 11:l:5005:PRO:HD2  | 1.93                     | 0.67              |
| 13:o:5141:ARG:HH11 | 13:o:5141:ARG:CG   | 2.07                     | 0.67              |
| 16:v:5054:GLU:O    | 16:v:5058:LEU:HD23 | 1.94                     | 0.67              |
| 1:A:160:ILE:HG21   | 3:C:431:PHE:CE1    | 2.30                     | 0.67              |
| 2:B:468:TRP:NE1    | 22:B:1019:CLA:HED2 | 2.09                     | 0.67              |
| 22:B:1009:CLA:O1A  | 22:B:1009:CLA:CHA  | 2.43                     | 0.67              |
| 3:C:166:ILE:HD12   | 3:C:249:ILE:CD1    | 2.22                     | 0.67              |
| 4:D:126:MET:HE2    | 4:D:143:ALA:O      | 1.94                     | 0.67              |
| 4:D:274:VAL:HG22   | 24:D:1042:PQ9:H293 | 1.76                     | 0.67              |
| 12:M:9:ILE:HD12    | 12:M:9:ILE:H       | 1.58                     | 0.67              |
| 13:O:188:ARG:HB2   | 13:O:188:ARG:NH1   | 2.09                     | 0.67              |
| 13:O:202:GLN:OE1   | 13:O:202:GLN:HA    | 1.93                     | 0.67              |
| 1:a:5089:ILE:HG21  | 1:a:5094:TYR:HB2   | 1.77                     | 0.67              |
| 1:a:5196:PRO:HG3   | 3:c:5404:LEU:CD1   | 2.23                     | 0.67              |
| 2:b:5235:GLU:HG2   | 2:b:5473:THR:HA    | 1.77                     | 0.67              |
| 2:b:5433:ASP:C     | 2:b:5433:ASP:OD1   | 2.37                     | 0.67              |
| 22:b:6009:CLA:O1A  | 22:b:6009:CLA:CHA  | 2.43                     | 0.67              |
| 3:c:5418:ASN:C     | 3:c:5418:ASN:OD1   | 2.38                     | 0.67              |
| 4:d:5043:LEU:HD23  | 4:d:5043:LEU:H     | 1.60                     | 0.67              |
| 10:k:5032:PHE:HE1  | 25:k:6052:BCR:C37  | 2.08                     | 0.67              |
| 22:k:6034:CLA:H43  | 22:k:6034:CLA:O1A  | 1.95                     | 0.67              |
| 18:y:5042:ARG:HB3  | 18:y:5043:ARG:NH1  | 2.10                     | 0.67              |
| 1:A:218:LEU:HA     | 1:A:221:SER:OG     | 1.95                     | 0.67              |
| 2:B:75:TRP:CD1     | 2:B:94:GLU:HB2     | 2.30                     | 0.67              |
| 22:B:1013:CLA:CAB  | 22:B:1014:CLA:C5   | 2.73                     | 0.67              |
| 3:C:453:ALA:HB2    | 8:I:31:ASN:ND2     | 2.10                     | 0.67              |
| 7:H:44:ILE:HD11    | 17:X:19:PHE:CD2    | 2.30                     | 0.67              |
| 8:I:12:VAL:O       | 8:I:16:VAL:HG23    | 1.95                     | 0.67              |
| 11:L:29:LEU:C      | 11:L:29:LEU:HD13   | 2.20                     | 0.67              |
| 15:U:83:THR:HG22   | 15:U:84:VAL:N      | 2.10                     | 0.67              |
| 1:a:5224:ILE:HG23  | 1:a:5225:ARG:N     | 2.08                     | 0.67              |
| 22:a:6007:CLA:CHA  | 22:a:6007:CLA:CBA  | 2.72                     | 0.67              |
| 13:o:5075:THR:HB   | 13:o:5262:GLN:HB2  | 1.77                     | 0.67              |
| 16:v:5105:PRO:HB2  | 16:v:5114:ILE:HG23 | 1.77                     | 0.67              |
| 1:A:64:ARG:HE      | 13:O:98:THR:HG21   | 1.59                     | 0.66              |
| 3:C:49:LEU:HD23    | 3:C:52:ALA:N       | 2.08                     | 0.66              |
| 3:C:187:ASP:HB2    | 3:C:230:LEU:CD1    | 2.25                     | 0.66              |
| 5:E:38:VAL:HG21    | 6:F:36:ALA:O       | 1.95                     | 0.66              |
| 1:a:5064:ARG:HE    | 13:o:5098:THR:HG21 | 1.59                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5150:PRO:CA    | 22:a:6003:CLA:H52  | 2.25                     | 0.66              |
| 2:b:5419:SER:HA    | 2:b:5422:ARG:NH1   | 2.10                     | 0.66              |
| 22:b:6012:CLA:CAB  | 22:b:6015:CLA:HBB2 | 2.24                     | 0.66              |
| 4:d:5068:LEU:HA    | 6:f:5040:MET:SD    | 2.35                     | 0.66              |
| 4:d:5110:LEU:O     | 4:d:5114:ILE:HG13  | 1.95                     | 0.66              |
| 24:d:6042:PQ9:H242 | 28:l:6061:MGE:CBB  | 2.25                     | 0.66              |
| 13:o:5082:PRO:HG2  | 13:o:5089:ALA:CB   | 2.24                     | 0.66              |
| 2:B:24:LEU:CD2     | 2:B:111:ALA:HA     | 2.25                     | 0.66              |
| 3:C:266:TRP:HB3    | 3:C:271:TYR:OH     | 1.94                     | 0.66              |
| 22:C:1029:CLA:O1A  | 22:C:1029:CLA:HBD  | 1.96                     | 0.66              |
| 22:D:1005:CLA:H122 | 28:D:1062:MGE:H263 | 1.78                     | 0.66              |
| 8:I:18:LEU:O       | 8:I:18:LEU:HD23    | 1.95                     | 0.66              |
| 22:K:1034:CLA:H43  | 22:K:1034:CLA:O1A  | 1.95                     | 0.66              |
| 1:a:5149:ALA:HB1   | 1:a:5283:VAL:CG1   | 2.24                     | 0.66              |
| 22:a:6003:CLA:H142 | 23:a:6038:PHO:C8   | 2.11                     | 0.66              |
| 2:b:5024:LEU:CD2   | 2:b:5111:ALA:HA    | 2.25                     | 0.66              |
| 3:c:5343:ARG:HG2   | 3:c:5348:GLU:O     | 1.94                     | 0.66              |
| 4:d:5100:ASP:O     | 4:d:5102:THR:N     | 2.28                     | 0.66              |
| 22:A:1003:CLA:H142 | 23:A:1038:PHO:C8   | 2.11                     | 0.66              |
| 2:B:451:PHE:CZ     | 22:B:1012:CLA:O1D  | 2.47                     | 0.66              |
| 4:D:44:ALA:HB1     | 23:D:1039:PHO:H102 | 1.77                     | 0.66              |
| 4:D:198:MET:SD     | 22:D:1005:CLA:CED  | 2.83                     | 0.66              |
| 4:D:350:ASN:O      | 4:D:351:ALA:HB2    | 1.95                     | 0.66              |
| 11:L:8:GLN:H       | 11:L:8:GLN:HE21    | 1.41                     | 0.66              |
| 13:O:172:PHE:HB2   | 13:O:221:GLY:N     | 2.08                     | 0.66              |
| 16:V:105:PRO:HB2   | 16:V:114:ILE:HG23  | 1.77                     | 0.66              |
| 1:a:5192:ILE:HD11  | 1:a:5293:MET:HE1   | 1.78                     | 0.66              |
| 1:a:5207:GLY:O     | 1:a:5210:LEU:N     | 2.27                     | 0.66              |
| 1:a:5310:LYS:HG2   | 16:v:5151:ILE:HG22 | 1.77                     | 0.66              |
| 2:b:5119:ASP:C     | 2:b:5120:LEU:HD23  | 2.20                     | 0.66              |
| 2:b:5226:TYR:HD2   | 2:b:5226:TYR:O     | 1.79                     | 0.66              |
| 22:b:6020:CLA:O2D  | 22:b:6020:CLA:H2A  | 1.95                     | 0.66              |
| 3:c:5405:ASN:O     | 3:c:5406:SER:HB2   | 1.94                     | 0.66              |
| 11:l:5021:LEU:CB   | 14:t:5016:LEU:HD21 | 2.24                     | 0.66              |
| 1:A:156:ALA:HB1    | 1:A:290:ILE:CG2    | 2.25                     | 0.66              |
| 1:A:210:LEU:HA     | 23:D:1039:PHO:HAC2 | 1.75                     | 0.66              |
| 23:A:1038:PHO:H201 | 22:D:1005:CLA:C3B  | 2.26                     | 0.66              |
| 22:B:1020:CLA:O2D  | 22:B:1020:CLA:H2A  | 1.95                     | 0.66              |
| 4:D:68:LEU:HA      | 6:F:40:MET:SD      | 2.35                     | 0.66              |
| 4:D:100:ASP:O      | 4:D:102:THR:N      | 2.28                     | 0.66              |
| 5:E:75:GLN:O       | 5:E:76:VAL:C       | 2.36                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:H:53:LEU:HD12    | 7:H:55:LEU:CD2     | 2.25                     | 0.66              |
| 15:U:25:ILE:HG21   | 15:U:35:PHE:HE2    | 1.59                     | 0.66              |
| 17:X:11:THR:HG23   | 17:X:11:THR:O      | 1.96                     | 0.66              |
| 1:a:5126:TYR:HD2   | 1:a:5126:TYR:C     | 2.03                     | 0.66              |
| 1:a:5156:ALA:HB1   | 1:a:5290:ILE:CG2   | 2.26                     | 0.66              |
| 1:a:5212:CYS:SG    | 4:d:5210:LEU:HB3   | 2.34                     | 0.66              |
| 2:b:5168:VAL:HG12  | 2:b:5169:SER:N     | 2.10                     | 0.66              |
| 2:b:5271:THR:HG22  | 2:b:5274:GLN:NE2   | 2.10                     | 0.66              |
| 2:b:5475:PHE:N     | 2:b:5475:PHE:CD2   | 2.62                     | 0.66              |
| 22:b:6022:CLA:H93  | 22:b:6022:CLA:H122 | 1.63                     | 0.66              |
| 3:c:5459:ILE:H     | 4:d:5224:GLN:H     | 1.44                     | 0.66              |
| 4:d:5045:LEU:HG    | 4:d:5049:LEU:HD12  | 1.76                     | 0.66              |
| 23:d:6039:PHO:HMA3 | 22:d:6004:CLA:H142 | 1.76                     | 0.66              |
| 22:d:6004:CLA:C20  | 28:d:6059:MGE:H8A1 | 2.26                     | 0.66              |
| 22:k:6034:CLA:CGD  | 22:k:6034:CLA:CAA  | 2.65                     | 0.66              |
| 11:l:5030:LEU:HD22 | 11:l:5031:PHE:CD1  | 2.30                     | 0.66              |
| 13:o:5188:ARG:NH1  | 13:o:5188:ARG:HB2  | 2.09                     | 0.66              |
| 16:v:5035:THR:HA   | 16:v:5046:THR:HA   | 1.77                     | 0.66              |
| 1:A:258:LEU:C      | 1:A:259:ILE:HG13   | 2.21                     | 0.66              |
| 2:B:119:ASP:C      | 2:B:120:LEU:HD23   | 2.20                     | 0.66              |
| 3:C:224:ILE:CD1    | 25:C:1054:BCR:H383 | 2.25                     | 0.66              |
| 3:C:298:PRO:O      | 3:C:299:SER:HB2    | 1.95                     | 0.66              |
| 18:Y:42:ARG:HB3    | 18:Y:43:ARG:NH1    | 2.10                     | 0.66              |
| 1:a:5214:MET:HE1   | 23:d:6039:PHO:O1D  | 1.95                     | 0.66              |
| 22:a:6006:CLA:C16  | 24:a:6043:PQ9:H443 | 2.22                     | 0.66              |
| 3:c:5295:THR:HG22  | 3:c:5296:VAL:N     | 2.11                     | 0.66              |
| 3:c:5318:LEU:HD21  | 3:c:5328:VAL:HG11  | 1.75                     | 0.66              |
| 4:d:5281:MET:HE2   | 4:d:5281:MET:CA    | 2.25                     | 0.66              |
| 23:d:6039:PHO:CHD  | 23:d:6039:PHO:CBC  | 2.74                     | 0.66              |
| 10:k:5032:PHE:CE1  | 25:k:6052:BCR:C37  | 2.78                     | 0.66              |
| 13:o:5086:ARG:HH11 | 13:o:5086:ARG:HG3  | 1.61                     | 0.66              |
| 23:A:1038:PHO:C20  | 22:D:1005:CLA:C3B  | 2.74                     | 0.66              |
| 2:B:475:PHE:CZ     | 4:D:134:ARG:HB2    | 2.31                     | 0.66              |
| 22:B:1022:CLA:H11  | 22:B:1022:CLA:CHA  | 2.25                     | 0.66              |
| 22:C:1030:CLA:HHC  | 22:C:1030:CLA:CBB  | 2.20                     | 0.66              |
| 11:L:30:LEU:HD22   | 11:L:31:PHE:CD1    | 2.30                     | 0.66              |
| 13:O:266:TYR:OH    | 13:O:268:SER:HB3   | 1.96                     | 0.66              |
| 15:U:46:ALA:HA     | 15:U:49:ILE:HD12   | 1.77                     | 0.66              |
| 18:Y:43:ARG:HD2    | 18:Y:44:GLY:H      | 1.60                     | 0.66              |
| 1:a:5267:ASN:HB3   | 1:a:5270:SER:OG    | 1.96                     | 0.66              |
| 22:a:6006:CLA:CBB  | 22:d:6004:CLA:C5   | 2.72                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5317:ASN:HA    | 2:b:5330:MET:HE1   | 1.77                     | 0.66              |
| 22:c:6025:CLA:O2A  | 22:c:6025:CLA:C3A  | 2.44                     | 0.66              |
| 22:c:6029:CLA:O1A  | 22:c:6029:CLA:HBD  | 1.96                     | 0.66              |
| 4:d:5267:LEU:HD23  | 4:d:5267:LEU:C     | 2.21                     | 0.66              |
| 7:h:5053:LEU:HD12  | 7:h:5055:LEU:CD2   | 2.25                     | 0.66              |
| 11:l:5029:LEU:HD13 | 11:l:5029:LEU:C    | 2.20                     | 0.66              |
| 17:x:5011:THR:O    | 17:x:5011:THR:HG23 | 1.95                     | 0.66              |
| 20:z:5043:GLY:O    | 20:z:5047:TRP:N    | 2.27                     | 0.66              |
| 1:A:90:GLY:HA2     | 1:A:167:SER:OG     | 1.95                     | 0.66              |
| 22:A:1003:CLA:HBC2 | 22:A:1003:CLA:CHD  | 2.25                     | 0.66              |
| 22:A:1006:CLA:CBB  | 22:D:1004:CLA:C5   | 2.72                     | 0.66              |
| 2:B:174:LEU:HD22   | 2:B:312:TYR:CZ     | 2.31                     | 0.66              |
| 3:C:63:TRP:NE1     | 22:C:1028:CLA:C2C  | 2.59                     | 0.66              |
| 22:D:1005:CLA:HAA2 | 24:D:1042:PQ9:H412 | 0.75                     | 0.66              |
| 24:D:1042:PQ9:H242 | 28:L:1061:MGE:CBB  | 2.25                     | 0.66              |
| 13:O:86:ARG:HG3    | 13:O:86:ARG:HH11   | 1.60                     | 0.66              |
| 2:b:5174:LEU:HD21  | 2:b:5312:TYR:CE1   | 2.31                     | 0.66              |
| 22:b:6019:CLA:H2A  | 22:b:6019:CLA:O1D  | 1.95                     | 0.66              |
| 3:c:5063:TRP:NE1   | 22:c:6028:CLA:C2C  | 2.59                     | 0.66              |
| 3:c:5166:ILE:HD13  | 3:c:5248:GLY:HA3   | 1.77                     | 0.66              |
| 1:A:62:GLY:HA2     | 1:A:87:ASN:HB2     | 1.76                     | 0.66              |
| 1:A:126:TYR:HD2    | 1:A:126:TYR:C      | 2.03                     | 0.66              |
| 3:C:151:TRP:HE3    | 3:C:157:MET:HE1    | 1.61                     | 0.66              |
| 3:C:405:ASN:O      | 3:C:406:SER:HB2    | 1.94                     | 0.66              |
| 3:C:418:ASN:C      | 3:C:418:ASN:OD1    | 2.38                     | 0.66              |
| 4:D:45:LEU:O       | 4:D:49:LEU:HD12    | 1.95                     | 0.66              |
| 13:O:196:SER:OG    | 13:O:197:ALA:N     | 2.26                     | 0.66              |
| 2:b:5012:LEU:O     | 2:b:5013:ILE:HG23  | 1.95                     | 0.66              |
| 2:b:5414:PRO:O     | 2:b:5418:LYS:HG3   | 1.96                     | 0.66              |
| 2:b:5468:TRP:NE1   | 22:b:6019:CLA:HED2 | 2.09                     | 0.66              |
| 22:b:6009:CLA:CGD  | 22:b:6009:CLA:CAA  | 2.74                     | 0.66              |
| 3:c:5151:TRP:HE3   | 3:c:5157:MET:HE1   | 1.61                     | 0.66              |
| 4:d:5045:LEU:O     | 4:d:5049:LEU:HD12  | 1.95                     | 0.66              |
| 4:d:5158:LEU:O     | 4:d:5162:LEU:HG    | 1.96                     | 0.66              |
| 4:d:5182:LEU:O     | 4:d:5183:LEU:C     | 2.37                     | 0.66              |
| 23:d:6039:PHO:O2A  | 23:d:6039:PHO:H42  | 1.95                     | 0.66              |
| 22:d:6004:CLA:H2A  | 22:d:6004:CLA:O1D  | 1.96                     | 0.66              |
| 1:A:104:GLU:OE2    | 13:O:99:ARG:HB3    | 1.96                     | 0.66              |
| 22:B:1009:CLA:HHC  | 22:B:1009:CLA:CBB  | 2.19                     | 0.66              |
| 29:B:1058:DGD:O2D  | 29:B:1058:DGD:HG31 | 1.94                     | 0.66              |
| 3:C:420:VAL:HB     | 3:C:425:TRP:NE1    | 2.09                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:267:LEU:HD23   | 4:D:267:LEU:C      | 2.21                     | 0.66              |
| 4:D:281:MET:HE2    | 4:D:281:MET:CA     | 2.25                     | 0.66              |
| 5:E:20:TRP:O       | 5:E:24:SER:HB3     | 1.95                     | 0.66              |
| 5:E:26:THR:O       | 5:E:29:ALA:HB3     | 1.96                     | 0.66              |
| 1:a:5064:ARG:NE    | 13:o:5098:THR:HG21 | 2.10                     | 0.66              |
| 1:a:5279:ARG:HG2   | 4:d:5212:ALA:HB2   | 1.75                     | 0.66              |
| 2:b:5334:ASP:HB3   | 13:o:5202:GLN:HG3  | 1.78                     | 0.66              |
| 2:b:5464:PHE:CE1   | 28:b:6060:MGE:H4B1 | 2.30                     | 0.66              |
| 3:c:5089:ILE:N     | 3:c:5090:PRO:HD2   | 2.11                     | 0.66              |
| 3:c:5224:ILE:CD1   | 25:c:6054:BCR:H383 | 2.25                     | 0.66              |
| 3:c:5240:ILE:HG13  | 22:c:6025:CLA:HAB  | 1.78                     | 0.66              |
| 3:c:5261:ARG:HA    | 3:c:5266:TRP:CZ2   | 2.30                     | 0.66              |
| 22:c:6028:CLA:H2A  | 22:c:6028:CLA:O1D  | 1.96                     | 0.66              |
| 7:h:5041:PHE:HD1   | 25:h:6049:BCR:H362 | 1.61                     | 0.66              |
| 1:A:37:MET:SD      | 1:A:126:TYR:HB2    | 2.36                     | 0.66              |
| 1:A:214:MET:HE1    | 23:D:1039:PHO:O1D  | 1.95                     | 0.66              |
| 2:B:414:PRO:O      | 2:B:418:LYS:HG3    | 1.96                     | 0.66              |
| 3:C:56:HIS:CD2     | 3:C:57:ALA:N       | 2.64                     | 0.66              |
| 3:C:295:THR:HG22   | 3:C:296:VAL:N      | 2.11                     | 0.66              |
| 22:C:1030:CLA:H121 | 22:C:1030:CLA:H171 | 1.72                     | 0.66              |
| 4:D:276:VAL:O      | 4:D:280:TRP:HD1    | 1.79                     | 0.66              |
| 14:T:11:ALA:CB     | 25:T:6046:BCR:H362 | 2.25                     | 0.66              |
| 1:a:5036:ILE:HD13  | 22:c:6029:CLA:H142 | 1.78                     | 0.66              |
| 1:a:5210:LEU:HD23  | 1:a:5210:LEU:O     | 1.96                     | 0.66              |
| 2:b:5055:MET:HE3   | 2:b:5080:ILE:HG21  | 1.78                     | 0.66              |
| 2:b:5075:TRP:CD1   | 2:b:5094:GLU:HB2   | 2.30                     | 0.66              |
| 3:c:5265:ILE:CD1   | 3:c:5452:ALA:CB    | 2.61                     | 0.66              |
| 3:c:5418:ASN:ND2   | 29:c:6057:DGD:HE61 | 2.11                     | 0.66              |
| 4:d:5029:PHE:CE2   | 4:d:5031:GLY:HA3   | 2.31                     | 0.66              |
| 4:d:5132:ILE:O     | 4:d:5136:VAL:HG23  | 1.96                     | 0.66              |
| 1:A:60:ILE:HG22    | 1:A:61:ASP:N       | 2.10                     | 0.65              |
| 1:A:93:PHE:HB2     | 3:C:218:PHE:HD2    | 1.62                     | 0.65              |
| 1:A:195:HIS:O      | 1:A:199:GLN:HG2    | 1.96                     | 0.65              |
| 22:B:1009:CLA:CGD  | 22:B:1009:CLA:CAA  | 2.74                     | 0.65              |
| 3:C:84:GLN:O       | 3:C:86:LEU:HG      | 1.95                     | 0.65              |
| 3:C:276:LEU:HD23   | 3:C:276:LEU:C      | 2.22                     | 0.65              |
| 22:C:1029:CLA:H52  | 22:C:1029:CLA:C1C  | 2.27                     | 0.65              |
| 4:D:43:LEU:HD23    | 4:D:43:LEU:H       | 1.59                     | 0.65              |
| 4:D:182:LEU:O      | 4:D:183:LEU:C      | 2.37                     | 0.65              |
| 15:U:42:TYR:HB3    | 15:U:43:PRO:CD     | 2.26                     | 0.65              |
| 1:a:5222:SER:C     | 2:b:5482:ILE:HG21  | 2.21                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5223:LEU:HD11  | 4:d:5265:ARG:HG2   | 1.78                     | 0.65              |
| 1:a:5258:LEU:C     | 1:a:5259:ILE:HG13  | 2.21                     | 0.65              |
| 2:b:5025:MET:HG3   | 25:b:6045:BCR:C40  | 2.25                     | 0.65              |
| 3:c:5056:HIS:CD2   | 3:c:5057:ALA:N     | 2.64                     | 0.65              |
| 3:c:5070:PHE:O     | 3:c:5073:ALA:HB3   | 1.96                     | 0.65              |
| 3:c:5257:PHE:H     | 3:c:5257:PHE:HD1   | 1.44                     | 0.65              |
| 4:d:5155:SER:HA    | 4:d:5159:ILE:HB    | 1.78                     | 0.65              |
| 5:e:5038:VAL:HG21  | 6:f:5036:ALA:O     | 1.95                     | 0.65              |
| 7:h:5044:ILE:HD11  | 17:x:5019:PHE:CD2  | 2.30                     | 0.65              |
| 2:B:168:VAL:HG12   | 2:B:169:SER:N      | 2.10                     | 0.65              |
| 2:B:475:PHE:N      | 2:B:475:PHE:CD2    | 2.62                     | 0.65              |
| 3:C:89:ILE:N       | 3:C:90:PRO:HD2     | 2.11                     | 0.65              |
| 22:C:1028:CLA:H2A  | 22:C:1028:CLA:O1D  | 1.96                     | 0.65              |
| 15:U:73:GLN:OE1    | 15:U:77:GLU:HG3    | 1.97                     | 0.65              |
| 16:V:61:TYR:O      | 16:V:129:LYS:HD3   | 1.96                     | 0.65              |
| 1:a:5214:MET:HE1   | 23:d:6039:PHO:CGD  | 2.26                     | 0.65              |
| 1:a:5218:LEU:HA    | 1:a:5221:SER:OG    | 1.95                     | 0.65              |
| 22:b:6021:CLA:HMA3 | 22:b:6021:CLA:C2   | 2.23                     | 0.65              |
| 3:c:5059:LEU:HD22  | 22:k:6034:CLA:HBD  | 1.77                     | 0.65              |
| 3:c:5084:GLN:O     | 3:c:5086:LEU:HG    | 1.95                     | 0.65              |
| 3:c:5298:PRO:O     | 3:c:5299:SER:HB2   | 1.95                     | 0.65              |
| 4:d:5044:ALA:HB1   | 23:d:6039:PHO:H102 | 1.77                     | 0.65              |
| 4:d:5312:GLU:OE1   | 13:o:5185:PRO:HB3  | 1.96                     | 0.65              |
| 4:d:5350:ASN:O     | 4:d:5351:ALA:HB2   | 1.95                     | 0.65              |
| 1:A:141:PRO:C      | 1:A:143:ILE:H      | 2.05                     | 0.65              |
| 1:A:205:VAL:HB     | 1:A:279:ARG:HH22   | 1.60                     | 0.65              |
| 2:B:317:ASN:HA     | 2:B:330:MET:HE1    | 1.77                     | 0.65              |
| 2:B:419:SER:HA     | 2:B:422:ARG:NH1    | 2.10                     | 0.65              |
| 3:C:63:TRP:NE1     | 22:C:1028:CLA:CMC  | 2.59                     | 0.65              |
| 3:C:257:PHE:HD1    | 3:C:257:PHE:H      | 1.44                     | 0.65              |
| 3:C:418:ASN:ND2    | 29:C:1057:DGD:HE61 | 2.11                     | 0.65              |
| 3:C:459:ILE:H      | 4:D:224:GLN:H      | 1.44                     | 0.65              |
| 15:U:43:PRO:HD3    | 16:V:108:TYR:HB3   | 1.78                     | 0.65              |
| 1:a:5090:GLY:HA2   | 1:a:5167:SER:OG    | 1.95                     | 0.65              |
| 22:b:6023:CLA:C13  | 22:b:6024:CLA:HMA1 | 2.23                     | 0.65              |
| 3:c:5453:ALA:HB2   | 8:i:5031:ASN:ND2   | 2.10                     | 0.65              |
| 22:c:6037:CLA:HBB1 | 22:c:6037:CLA:CHC  | 2.14                     | 0.65              |
| 4:d:5182:LEU:O     | 4:d:5185:PHE:N     | 2.29                     | 0.65              |
| 14:t:5017:PHE:O    | 14:t:5021:ILE:HG13 | 1.96                     | 0.65              |
| 15:u:5083:THR:HG22 | 15:u:5084:VAL:N    | 2.10                     | 0.65              |
| 1:A:64:ARG:NE      | 13:O:98:THR:HG21   | 2.10                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:207:GLY:O      | 1:A:210:LEU:N      | 2.27                     | 0.65              |
| 1:A:247:ASN:HD21   | 2:B:486:LEU:HB3    | 1.59                     | 0.65              |
| 3:C:166:ILE:HD13   | 3:C:248:GLY:HA3    | 1.77                     | 0.65              |
| 22:C:1029:CLA:HBA1 | 8:I:23:PHE:CE1     | 2.32                     | 0.65              |
| 29:C:1055:DGD:CEB  | 29:C:1055:DGD:HBG3 | 2.25                     | 0.65              |
| 5:E:79:PHE:O       | 5:E:83:LEU:HB2     | 1.95                     | 0.65              |
| 12:M:8:PHE:HB3     | 12:m:5009:ILE:CG1  | 2.27                     | 0.65              |
| 13:O:59:ASP:OD1    | 13:O:61:SER:HB2    | 1.96                     | 0.65              |
| 15:U:28:ASN:HD21   | 15:U:55:TYR:N      | 1.95                     | 0.65              |
| 1:a:5039:PRO:HB2   | 22:a:6007:CLA:CBB  | 2.27                     | 0.65              |
| 1:a:5160:ILE:HG21  | 3:c:5431:PHE:CE1   | 2.30                     | 0.65              |
| 2:b:5165:GLY:HA3   | 2:b:5179:GLN:O     | 1.96                     | 0.65              |
| 22:b:6021:CLA:CED  | 22:b:6021:CLA:CHA  | 2.61                     | 0.65              |
| 3:c:5063:TRP:NE1   | 22:c:6028:CLA:CMC  | 2.59                     | 0.65              |
| 7:h:5013:PRO:HG2   | 7:h:5014:LEU:CD1   | 2.22                     | 0.65              |
| 25:t:1046:BCR:H323 | 25:t:1046:BCR:HC41 | 1.77                     | 0.65              |
| 16:v:5081:ARG:HG3  | 16:v:5157:GLY:HA3  | 1.78                     | 0.65              |
| 1:A:252:HIS:NE2    | 1:A:264:SER:HB3    | 2.12                     | 0.65              |
| 3:C:348:GLU:HB3    | 13:O:42:ALA:HB3    | 1.79                     | 0.65              |
| 22:C:1033:CLA:H2   | 22:C:1033:CLA:C7   | 2.27                     | 0.65              |
| 4:D:350:ASN:O      | 4:D:351:ALA:CB     | 2.44                     | 0.65              |
| 13:O:107:ILE:CG2   | 13:O:123:GLU:HG3   | 2.26                     | 0.65              |
| 13:O:250:ASP:HB3   | 13:O:253:ALA:HB3   | 1.78                     | 0.65              |
| 14:T:17:PHE:O      | 14:T:21:ILE:HG13   | 1.96                     | 0.65              |
| 1:a:5013:LEU:HD12  | 1:a:5013:LEU:N     | 2.12                     | 0.65              |
| 2:b:5475:PHE:CZ    | 4:d:5134:ARG:HB2   | 2.31                     | 0.65              |
| 22:b:6023:CLA:C4C  | 22:b:6024:CLA:HBC2 | 2.26                     | 0.65              |
| 3:c:5050:LEU:CD2   | 3:c:5054:VAL:HG23  | 2.25                     | 0.65              |
| 4:d:5090:LEU:HD12  | 4:d:5096:GLU:HG3   | 1.79                     | 0.65              |
| 4:d:5276:VAL:O     | 4:d:5280:TRP:HD1   | 1.79                     | 0.65              |
| 5:e:5026:THR:O     | 5:e:5029:ALA:HB3   | 1.96                     | 0.65              |
| 13:o:5250:ASP:HB3  | 13:o:5253:ALA:HB3  | 1.78                     | 0.65              |
| 15:u:5042:TYR:HB3  | 15:u:5043:PRO:HD2  | 1.78                     | 0.65              |
| 1:A:36:ILE:HD13    | 22:C:1029:CLA:C14  | 2.27                     | 0.65              |
| 2:B:334:ASP:HB3    | 13:O:202:GLN:HG3   | 1.78                     | 0.65              |
| 2:B:464:PHE:CE1    | 28:B:1060:MGE:H4B1 | 2.30                     | 0.65              |
| 22:B:1023:CLA:C4C  | 22:B:1024:CLA:HBC2 | 2.26                     | 0.65              |
| 3:C:428:THR:CG2    | 3:C:429:SER:N      | 2.57                     | 0.65              |
| 1:a:5036:ILE:HD13  | 22:c:6029:CLA:C14  | 2.27                     | 0.65              |
| 1:a:5279:ARG:HD3   | 4:d:5208:ALA:CB    | 2.25                     | 0.65              |
| 22:a:6006:CLA:HBB1 | 22:a:6006:CLA:CHC  | 2.19                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6011:CLA:HMD1 | 22:b:6014:CLA:CAB  | 2.27                     | 0.65              |
| 22:b:6012:CLA:H43  | 22:b:6013:CLA:H41  | 1.79                     | 0.65              |
| 3:c:5396:MET:CE    | 16:v:5074:THR:HA   | 2.26                     | 0.65              |
| 22:c:6029:CLA:H52  | 22:c:6029:CLA:C1C  | 2.27                     | 0.65              |
| 4:d:5350:ASN:O     | 4:d:5351:ALA:CB    | 2.44                     | 0.65              |
| 8:i:5018:LEU:HD23  | 8:i:5018:LEU:O     | 1.95                     | 0.65              |
| 15:u:5073:GLN:OE1  | 15:u:5077:GLU:HG3  | 1.97                     | 0.65              |
| 1:A:186:PHE:O      | 1:A:187:GLN:C      | 2.40                     | 0.65              |
| 1:A:187:GLN:HG3    | 1:A:325:ASN:ND2    | 2.10                     | 0.65              |
| 1:A:222:SER:C      | 2:B:482:ILE:HG21   | 2.21                     | 0.65              |
| 4:D:29:PHE:CE2     | 4:D:31:GLY:HA3     | 2.31                     | 0.65              |
| 4:D:90:LEU:HD12    | 4:D:96:GLU:HG3     | 1.79                     | 0.65              |
| 16:V:66:CYS:SG     | 31:V:1041:HEM:CAC  | 2.85                     | 0.65              |
| 1:a:5212:CYS:CB    | 4:d:5211:CYS:HB2   | 2.24                     | 0.65              |
| 23:a:6038:PHO:C20  | 22:d:6005:CLA:C3B  | 2.74                     | 0.65              |
| 2:b:5357:ARG:HG2   | 2:b:5357:ARG:NH1   | 2.09                     | 0.65              |
| 22:b:6009:CLA:O1A  | 22:b:6009:CLA:NA   | 2.30                     | 0.65              |
| 22:b:6016:CLA:HBC3 | 22:b:6016:CLA:CHD  | 2.26                     | 0.65              |
| 4:d:5207:GLY:HA2   | 4:d:5274:VAL:HG11  | 1.79                     | 0.65              |
| 22:d:6005:CLA:C9   | 22:d:6005:CLA:H121 | 2.26                     | 0.65              |
| 13:o:5107:ILE:CG2  | 13:o:5123:GLU:HG3  | 2.26                     | 0.65              |
| 14:t:5020:ALA:O    | 14:t:5024:ARG:HB3  | 1.96                     | 0.65              |
| 1:A:192:ILE:HD11   | 1:A:293:MET:HE1    | 1.78                     | 0.65              |
| 1:A:214:MET:HE1    | 23:D:1039:PHO:CGD  | 2.27                     | 0.65              |
| 1:A:279:ARG:HE     | 23:A:1038:PHO:C2C  | 2.10                     | 0.65              |
| 2:B:165:GLY:HA3    | 2:B:179:GLN:O      | 1.96                     | 0.65              |
| 2:B:226:TYR:O      | 2:B:226:TYR:HD2    | 1.79                     | 0.65              |
| 3:C:263:ALA:CB     | 3:C:264:PHE:HD2    | 2.10                     | 0.65              |
| 3:C:275:SER:CB     | 22:C:1033:CLA:HED1 | 2.20                     | 0.65              |
| 25:C:1052:BCR:H361 | 10:K:32:PHE:CE2    | 2.31                     | 0.65              |
| 22:D:1004:CLA:H2A  | 22:D:1004:CLA:O1D  | 1.96                     | 0.65              |
| 15:U:68:THR:HG22   | 15:U:71:GLN:N      | 2.10                     | 0.65              |
| 1:a:5141:PRO:C     | 1:a:5143:ILE:H     | 2.05                     | 0.65              |
| 1:a:5259:ILE:H     | 4:d:5128:ARG:HH22  | 1.43                     | 0.65              |
| 1:a:5272:HIS:HB3   | 4:d:5218:VAL:HG11  | 1.79                     | 0.65              |
| 3:c:5100:GLY:HA2   | 3:c:5196:VAL:CG1   | 2.23                     | 0.65              |
| 3:c:5334:PRO:HD3   | 3:c:5339:LYS:HE3   | 1.79                     | 0.65              |
| 22:c:6031:CLA:H2   | 22:c:6031:CLA:HMA3 | 1.78                     | 0.65              |
| 15:u:5042:TYR:HB3  | 15:u:5043:PRO:CD   | 2.26                     | 0.65              |
| 16:v:5032:GLU:HA   | 16:v:5035:THR:OG1  | 1.97                     | 0.65              |
| 16:v:5098:LEU:HD22 | 16:v:5098:LEU:N    | 2.03                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:13:LEU:HD12    | 1:A:13:LEU:N       | 2.12                     | 0.65              |
| 1:A:210:LEU:HD23   | 1:A:210:LEU:O      | 1.96                     | 0.65              |
| 1:A:267:ASN:HB3    | 1:A:270:SER:OG     | 1.96                     | 0.65              |
| 2:B:90:PHE:C       | 2:B:90:PHE:CD2     | 2.75                     | 0.65              |
| 22:B:1009:CLA:O1A  | 22:B:1009:CLA:NA   | 2.30                     | 0.65              |
| 3:C:50:LEU:HD22    | 3:C:51:GLY:N       | 2.12                     | 0.65              |
| 3:C:334:PRO:HD3    | 3:C:339:LYS:HE3    | 1.79                     | 0.65              |
| 22:C:1030:CLA:HED3 | 22:C:1030:CLA:CHA  | 2.27                     | 0.65              |
| 29:C:1056:DGD:HBF2 | 29:C:1056:DGD:HGB2 | 0.81                     | 0.65              |
| 22:D:1004:CLA:C20  | 28:D:1059:MGE:H8A1 | 2.26                     | 0.65              |
| 24:D:1042:PQ9:H241 | 28:L:1061:MGE:H263 | 1.79                     | 0.65              |
| 10:K:28:ILE:O      | 10:K:29:PRO:C      | 2.36                     | 0.65              |
| 22:K:1034:CLA:HHD  | 22:K:1034:CLA:CBC  | 2.17                     | 0.65              |
| 14:T:24:ARG:HD2    | 14:T:24:ARG:O      | 1.97                     | 0.65              |
| 1:a:5195:HIS:O     | 1:a:5199:GLN:HG2   | 1.96                     | 0.65              |
| 1:a:5309:ALA:HB3   | 16:v:5028:GLU:HB2  | 1.79                     | 0.65              |
| 26:a:6063:LHG:HC41 | 3:c:5036:TRP:CH2   | 2.31                     | 0.65              |
| 2:b:5069:LEU:HD21  | 22:b:6013:CLA:O1A  | 1.97                     | 0.65              |
| 22:b:6013:CLA:CAB  | 22:b:6014:CLA:C5   | 2.73                     | 0.65              |
| 3:c:5172:ALA:O     | 3:c:5176:VAL:HG23  | 1.97                     | 0.65              |
| 3:c:5450:ALA:HB3   | 3:c:5456:GLU:HB3   | 1.79                     | 0.65              |
| 31:f:6040:HEM:CMA  | 31:f:6040:HEM:CBA  | 2.61                     | 0.65              |
| 13:o:5059:ASP:OD1  | 13:o:5061:SER:HB2  | 1.96                     | 0.65              |
| 26:A:1063:LHG:HC41 | 3:C:36:TRP:CH2     | 2.31                     | 0.65              |
| 2:B:235:GLU:HG2    | 2:B:473:THR:HA     | 1.77                     | 0.65              |
| 3:C:281:MET:O      | 3:C:285:ILE:HG13   | 1.97                     | 0.65              |
| 3:C:282:MET:SD     | 22:C:1025:CLA:H71  | 2.37                     | 0.65              |
| 3:C:333:GLY:H      | 3:C:338:GLY:CA     | 2.10                     | 0.65              |
| 29:C:1056:DGD:HBF1 | 29:C:1056:DGD:HB92 | 1.77                     | 0.65              |
| 4:D:184:PHE:CE2    | 4:D:188:PHE:HD1    | 2.11                     | 0.65              |
| 7:H:41:PHE:HD1     | 25:H:1049:BCR:H362 | 1.61                     | 0.65              |
| 16:V:94:ASN:C      | 16:V:96:GLU:N      | 2.52                     | 0.65              |
| 1:a:5116:ILE:CD1   | 1:a:5158:PHE:HB3   | 2.27                     | 0.65              |
| 1:a:5119:PHE:C     | 1:a:5119:PHE:CD2   | 2.75                     | 0.65              |
| 2:b:5103:LEU:HD12  | 2:b:5107:LEU:HG    | 1.79                     | 0.65              |
| 2:b:5174:LEU:HD22  | 2:b:5312:TYR:CZ    | 2.31                     | 0.65              |
| 3:c:5276:LEU:HD23  | 3:c:5276:LEU:C     | 2.22                     | 0.65              |
| 22:c:6033:CLA:HBB1 | 22:c:6033:CLA:CHC  | 2.26                     | 0.65              |
| 4:d:5194:ASN:O     | 4:d:5198:MET:HG3   | 1.97                     | 0.65              |
| 4:d:5217:THR:HG21  | 24:d:6042:PQ9:O4   | 1.96                     | 0.65              |
| 22:k:6034:CLA:H91  | 22:k:6034:CLA:H121 | 1.79                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:t:1046:BCR:C23  | 25:t:1046:BCR:H403 | 2.27                     | 0.65              |
| 16:v:5061:TYR:O    | 16:v:5129:LYS:HD3  | 1.96                     | 0.65              |
| 1:A:89:ILE:HG21    | 1:A:94:TYR:HB2     | 1.77                     | 0.64              |
| 1:A:259:ILE:H      | 4:D:128:ARG:HH22   | 1.43                     | 0.64              |
| 1:A:310:LYS:HG2    | 16:V:151:ILE:HG22  | 1.77                     | 0.64              |
| 2:B:454:ALA:C      | 2:B:456:ALA:H      | 2.05                     | 0.64              |
| 3:C:171:GLY:CA     | 22:C:1025:CLA:HBC1 | 2.27                     | 0.64              |
| 22:C:1025:CLA:O2A  | 22:C:1025:CLA:C3A  | 2.44                     | 0.64              |
| 4:D:132:ILE:O      | 4:D:136:VAL:HG23   | 1.96                     | 0.64              |
| 4:D:222:LEU:HD23   | 4:D:243:THR:O      | 1.98                     | 0.64              |
| 13:O:83:LYS:HE3    | 2:b:5049:ASP:HB2   | 1.79                     | 0.64              |
| 14:T:20:ALA:O      | 14:T:24:ARG:HB3    | 1.96                     | 0.64              |
| 1:a:5252:HIS:NE2   | 1:a:5264:SER:HB3   | 2.12                     | 0.64              |
| 3:c:5428:THR:CG2   | 3:c:5429:SER:N     | 2.57                     | 0.64              |
| 4:d:5201:VAL:O     | 4:d:5205:LEU:HB3   | 1.97                     | 0.64              |
| 22:d:6005:CLA:H122 | 28:d:6062:MGE:H263 | 1.78                     | 0.64              |
| 22:d:6005:CLA:H92  | 22:d:6005:CLA:H121 | 1.79                     | 0.64              |
| 10:k:5032:PHE:O    | 10:k:5034:ALA:N    | 2.30                     | 0.64              |
| 13:o:5092:VAL:CG1  | 13:o:5093:PRO:HD2  | 2.27                     | 0.64              |
| 13:o:5266:TYR:OH   | 13:o:5268:SER:HB3  | 1.96                     | 0.64              |
| 15:u:5043:PRO:HD3  | 16:v:5108:TYR:HB3  | 1.78                     | 0.64              |
| 20:z:5020:VAL:O    | 20:z:5024:PRO:CD   | 2.45                     | 0.64              |
| 1:A:150:PRO:CA     | 22:A:1003:CLA:H52  | 2.25                     | 0.64              |
| 4:D:217:THR:HG21   | 24:D:1042:PQ9:O4   | 1.96                     | 0.64              |
| 22:D:1005:CLA:H152 | 22:D:1005:CLA:H202 | 1.79                     | 0.64              |
| 23:D:1039:PHO:CHD  | 23:D:1039:PHO:CBC  | 2.74                     | 0.64              |
| 5:E:13:ILE:HG13    | 5:E:19:TYR:HB2     | 1.79                     | 0.64              |
| 13:O:75:THR:HB     | 13:O:262:GLN:HB2   | 1.77                     | 0.64              |
| 1:a:5104:GLU:OE2   | 13:o:5099:ARG:HB3  | 1.96                     | 0.64              |
| 1:a:5192:ILE:HG12  | 1:a:5293:MET:SD    | 2.37                     | 0.64              |
| 2:b:5090:PHE:C     | 2:b:5090:PHE:CD2   | 2.75                     | 0.64              |
| 2:b:5280:PHE:O     | 2:b:5284:ILE:HG13  | 1.96                     | 0.64              |
| 16:v:5066:CYS:SG   | 31:v:6041:HEM:CAC  | 2.85                     | 0.64              |
| 18:y:5039:LEU:HD21 | 20:z:5028:ALA:CB   | 2.27                     | 0.64              |
| 1:A:36:ILE:HD13    | 22:C:1029:CLA:H142 | 1.78                     | 0.64              |
| 2:B:174:LEU:HD21   | 2:B:312:TYR:CE1    | 2.31                     | 0.64              |
| 3:C:50:LEU:CD2     | 3:C:54:VAL:HG23    | 2.26                     | 0.64              |
| 3:C:70:PHE:O       | 3:C:73:ALA:HB3     | 1.96                     | 0.64              |
| 3:C:223:TRP:HE1    | 3:C:224:ILE:HG12   | 1.62                     | 0.64              |
| 3:C:240:ILE:HG13   | 22:C:1025:CLA:HAB  | 1.78                     | 0.64              |
| 4:D:312:GLU:OE1    | 13:O:185:PRO:HB3   | 1.96                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:T:18:PHE:CA     | 25:T:6046:BCR:C33  | 2.74                     | 0.64              |
| 16:V:81:ARG:HG3    | 16:V:157:GLY:HA3   | 1.78                     | 0.64              |
| 1:a:5037:MET:SD    | 1:a:5126:TYR:HB2   | 2.37                     | 0.64              |
| 23:a:6038:PHO:H201 | 22:d:6005:CLA:C3B  | 2.26                     | 0.64              |
| 3:c:5050:LEU:HD22  | 3:c:5051:GLY:N     | 2.12                     | 0.64              |
| 13:o:5129:PHE:O    | 13:o:5129:PHE:CD2  | 2.50                     | 0.64              |
| 3:C:396:MET:CE     | 16:V:74:THR:HA     | 2.26                     | 0.64              |
| 3:C:450:ALA:HB3    | 3:C:456:GLU:HB3    | 1.79                     | 0.64              |
| 4:D:158:LEU:O      | 4:D:162:LEU:HG     | 1.96                     | 0.64              |
| 22:H:1017:CLA:HBB1 | 25:H:1049:BCR:H322 | 1.79                     | 0.64              |
| 25:K:1051:BCR:H351 | 25:K:1051:BCR:C16  | 2.26                     | 0.64              |
| 25:T:6046:BCR:H403 | 25:T:6046:BCR:C23  | 2.27                     | 0.64              |
| 1:a:5186:PHE:O     | 1:a:5187:GLN:C     | 2.40                     | 0.64              |
| 2:b:5063:LEU:N     | 2:b:5064:PRO:CD    | 2.61                     | 0.64              |
| 22:c:6029:CLA:HBA1 | 8:i:5023:PHE:CE1   | 2.32                     | 0.64              |
| 25:k:6051:BCR:H351 | 25:k:6051:BCR:C16  | 2.26                     | 0.64              |
| 11:l:5029:LEU:HD13 | 11:l:5029:LEU:O    | 1.98                     | 0.64              |
| 22:B:1011:CLA:CGA  | 22:B:1011:CLA:H42  | 2.28                     | 0.64              |
| 22:B:1011:CLA:HMD1 | 22:B:1014:CLA:CAB  | 2.27                     | 0.64              |
| 22:C:1025:CLA:H143 | 25:C:1054:BCR:H353 | 1.80                     | 0.64              |
| 1:a:5323:ARG:NE    | 4:d:5332:GLN:NE2   | 2.46                     | 0.64              |
| 2:b:5137:LYS:O     | 2:b:5138:MET:C     | 2.41                     | 0.64              |
| 22:c:6025:CLA:C1   | 22:c:6025:CLA:C4A  | 2.76                     | 0.64              |
| 5:e:5008:ARG:HE    | 6:f:5013:TYR:CB    | 2.02                     | 0.64              |
| 5:e:5017:VAL:O     | 5:e:5021:VAL:HG23  | 1.98                     | 0.64              |
| 25:h:6049:BCR:H23C | 25:h:6049:BCR:H393 | 1.71                     | 0.64              |
| 25:k:6051:BCR:C35  | 18:y:5032:GLY:HA3  | 2.20                     | 0.64              |
| 18:y:5043:ARG:HD2  | 18:y:5044:GLY:H    | 1.60                     | 0.64              |
| 1:A:159:LEU:HD21   | 29:C:1055:DGD:C7A  | 2.26                     | 0.64              |
| 2:B:69:LEU:HD21    | 22:B:1013:CLA:O1A  | 1.97                     | 0.64              |
| 2:B:372:ASP:HB3    | 2:B:376:VAL:HB     | 1.79                     | 0.64              |
| 28:B:1060:MGE:CBB  | 28:B:1060:MGE:H263 | 2.28                     | 0.64              |
| 3:C:81:MET:HG3     | 3:C:86:LEU:HD12    | 1.79                     | 0.64              |
| 22:D:1005:CLA:C9   | 22:D:1005:CLA:H121 | 2.26                     | 0.64              |
| 22:D:1005:CLA:H92  | 22:D:1005:CLA:H121 | 1.79                     | 0.64              |
| 18:Y:43:ARG:HD3    | 20:Z:31:GLN:HE21   | 1.63                     | 0.64              |
| 3:c:5049:LEU:CD2   | 3:c:5052:ALA:CA    | 2.76                     | 0.64              |
| 3:c:5081:MET:HG3   | 3:c:5086:LEU:HD12  | 1.79                     | 0.64              |
| 22:c:6033:CLA:H2   | 22:c:6033:CLA:C7   | 2.27                     | 0.64              |
| 22:c:6033:CLA:H91  | 22:c:6036:CLA:CAA  | 2.27                     | 0.64              |
| 13:o:5148:VAL:HG23 | 13:o:5172:PHE:CE2  | 2.33                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:t:5024:ARG:HD2  | 14:t:5024:ARG:O    | 1.97                     | 0.64              |
| 16:v:5038:LEU:HA   | 16:v:5095:ILE:CG2  | 2.26                     | 0.64              |
| 1:A:223:LEU:HD11   | 4:D:265:ARG:HG2    | 1.78                     | 0.64              |
| 22:B:1016:CLA:HBC3 | 22:B:1016:CLA:CHD  | 2.26                     | 0.64              |
| 3:C:172:ALA:O      | 3:C:176:VAL:HG23   | 1.97                     | 0.64              |
| 3:C:229:ASN:H      | 3:C:229:ASN:ND2    | 1.85                     | 0.64              |
| 22:C:1033:CLA:H91  | 22:C:1036:CLA:CAA  | 2.27                     | 0.64              |
| 4:D:207:GLY:HA2    | 4:D:274:VAL:HG11   | 1.79                     | 0.64              |
| 7:H:13:PRO:HG2     | 7:H:14:LEU:CD1     | 2.22                     | 0.64              |
| 7:H:54:ILE:C       | 7:H:55:LEU:HD22    | 2.23                     | 0.64              |
| 13:O:92:VAL:CG1    | 13:O:93:PRO:HD2    | 2.27                     | 0.64              |
| 15:U:42:TYR:HB3    | 15:U:43:PRO:HD2    | 1.78                     | 0.64              |
| 15:U:53:ALA:HB1    | 15:U:54:PRO:HD2    | 1.79                     | 0.64              |
| 3:c:5281:MET:O     | 3:c:5285:ILE:HG13  | 1.97                     | 0.64              |
| 22:c:6030:CLA:HHC  | 22:c:6030:CLA:CBB  | 2.20                     | 0.64              |
| 22:c:6033:CLA:O1A  | 22:c:6033:CLA:C2   | 2.45                     | 0.64              |
| 4:d:5222:LEU:HD23  | 4:d:5243:THR:O     | 1.98                     | 0.64              |
| 8:i:5004:LEU:O     | 8:i:5008:VAL:HG22  | 1.97                     | 0.64              |
| 1:A:39:PRO:HB2     | 22:A:1007:CLA:CBB  | 2.27                     | 0.64              |
| 22:B:1012:CLA:H43  | 22:B:1013:CLA:H41  | 1.79                     | 0.64              |
| 3:C:49:LEU:CD2     | 3:C:52:ALA:CA      | 2.76                     | 0.64              |
| 3:C:374:GLY:HA2    | 13:O:33:TYR:CD1    | 2.33                     | 0.64              |
| 22:C:1031:CLA:H2   | 22:C:1031:CLA:HMA3 | 1.78                     | 0.64              |
| 4:D:91:LEU:HG      | 22:D:1008:CLA:HED2 | 1.79                     | 0.64              |
| 4:D:279:LEU:HD21   | 23:D:1039:PHO:HMC1 | 1.80                     | 0.64              |
| 12:M:9:ILE:HD12    | 12:m:5009:ILE:CD1  | 2.18                     | 0.64              |
| 1:a:5093:PHE:HB2   | 3:c:5218:PHE:HD2   | 1.61                     | 0.64              |
| 2:b:5030:VAL:HG13  | 22:b:6013:CLA:HMD1 | 1.79                     | 0.64              |
| 2:b:5454:ALA:C     | 2:b:5456:ALA:H     | 2.05                     | 0.64              |
| 3:c:5274:TYR:HE1   | 22:c:6029:CLA:O1D  | 1.81                     | 0.64              |
| 3:c:5282:MET:SD    | 22:c:6025:CLA:H71  | 2.37                     | 0.64              |
| 22:c:6029:CLA:C4   | 22:c:6029:CLA:C1C  | 2.75                     | 0.64              |
| 22:c:6032:CLA:HBC2 | 22:c:6032:CLA:HHD  | 1.79                     | 0.64              |
| 7:h:5054:ILE:C     | 7:h:5055:LEU:HD22  | 2.23                     | 0.64              |
| 1:A:126:TYR:C      | 1:A:126:TYR:CD2    | 2.76                     | 0.64              |
| 2:B:137:LYS:O      | 2:B:138:MET:C      | 2.41                     | 0.64              |
| 2:B:173:GLY:HA3    | 2:B:174:LEU:C      | 2.23                     | 0.64              |
| 2:B:280:PHE:O      | 2:B:284:ILE:HG13   | 1.96                     | 0.64              |
| 22:B:1015:CLA:H122 | 22:B:1015:CLA:H91  | 1.80                     | 0.64              |
| 22:B:1021:CLA:H2   | 22:B:1021:CLA:HED1 | 1.79                     | 0.64              |
| 22:C:1033:CLA:O1A  | 22:C:1033:CLA:C2   | 2.45                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:C:1055:DGD:HAT1 | 29:C:1055:DGD:HA61 | 1.78                     | 0.64              |
| 15:U:68:THR:HG22   | 15:U:71:GLN:CB     | 2.28                     | 0.64              |
| 22:a:6003:CLA:HBC2 | 22:a:6003:CLA:CHD  | 2.25                     | 0.64              |
| 3:c:5318:LEU:HD23  | 3:c:5318:LEU:O     | 1.98                     | 0.64              |
| 3:c:5374:GLY:HA2   | 13:o:5033:TYR:CD1  | 2.33                     | 0.64              |
| 22:c:6033:CLA:HMA1 | 22:k:6034:CLA:C3C  | 2.25                     | 0.64              |
| 29:c:6056:DGD:HB1  | 29:c:6056:DGD:HB92 | 1.77                     | 0.64              |
| 4:d:5091:LEU:HG    | 22:d:6008:CLA:HED2 | 1.79                     | 0.64              |
| 22:A:1007:CLA:H2A  | 22:A:1007:CLA:O1D  | 1.98                     | 0.64              |
| 2:B:30:VAL:HG13    | 22:B:1013:CLA:HMD1 | 1.80                     | 0.64              |
| 2:B:178:VAL:O      | 2:B:178:VAL:HG13   | 1.99                     | 0.64              |
| 2:B:249:ALA:O      | 2:B:252:VAL:N      | 2.31                     | 0.64              |
| 22:B:1011:CLA:O1A  | 22:B:1011:CLA:H42  | 1.98                     | 0.64              |
| 22:C:1029:CLA:C4   | 22:C:1029:CLA:C1C  | 2.75                     | 0.64              |
| 4:D:145:ALA:HB2    | 4:D:272:LEU:CD1    | 2.28                     | 0.64              |
| 10:K:21:LEU:HD11   | 18:Y:24:MET:CG     | 2.27                     | 0.64              |
| 13:O:148:VAL:HG23  | 13:O:172:PHE:CE2   | 2.33                     | 0.64              |
| 25:T:6048:BCR:H342 | 22:b:6014:CLA:C9   | 2.28                     | 0.64              |
| 2:b:5030:VAL:CG1   | 22:b:6013:CLA:HMD1 | 2.28                     | 0.64              |
| 2:b:5097:ALA:C     | 2:b:5099:ALA:N     | 2.54                     | 0.64              |
| 22:b:6009:CLA:HBB1 | 22:b:6009:CLA:CHC  | 2.16                     | 0.64              |
| 3:c:5171:GLY:CA    | 22:c:6025:CLA:HBC1 | 2.27                     | 0.64              |
| 6:f:5034:LEU:HD12  | 9:j:5024:ILE:CD1   | 2.28                     | 0.64              |
| 13:o:5104:LEU:HD12 | 13:o:5104:LEU:O    | 1.98                     | 0.64              |
| 15:u:5063:ASN:O    | 15:u:5063:ASN:ND2  | 2.31                     | 0.64              |
| 1:A:150:PRO:HA     | 22:A:1003:CLA:H52  | 1.81                     | 0.63              |
| 22:B:1023:CLA:C13  | 22:B:1024:CLA:HMA1 | 2.23                     | 0.63              |
| 3:C:274:TYR:HE1    | 22:C:1029:CLA:O1D  | 1.81                     | 0.63              |
| 22:C:1025:CLA:C1   | 22:C:1025:CLA:C4A  | 2.76                     | 0.63              |
| 22:K:1034:CLA:H121 | 22:K:1034:CLA:H91  | 1.79                     | 0.63              |
| 16:V:32:GLU:HA     | 16:V:35:THR:OG1    | 1.97                     | 0.63              |
| 22:a:6006:CLA:CBC  | 22:a:6006:CLA:CHD  | 2.74                     | 0.63              |
| 2:b:5023:HIS:O     | 2:b:5027:THR:HB    | 1.98                     | 0.63              |
| 2:b:5173:GLY:HA3   | 2:b:5174:LEU:C     | 2.23                     | 0.63              |
| 22:b:6022:CLA:H121 | 12:m:5024:ILE:HD12 | 1.80                     | 0.63              |
| 3:c:5170:ILE:HG22  | 3:c:5171:GLY:N     | 2.13                     | 0.63              |
| 22:c:6025:CLA:H143 | 25:c:6054:BCR:H353 | 1.79                     | 0.63              |
| 22:c:6031:CLA:H2A  | 22:c:6031:CLA:O2D  | 1.98                     | 0.63              |
| 4:d:5123:ILE:O     | 4:d:5127:LEU:HG    | 1.97                     | 0.63              |
| 13:o:5152:VAL:O    | 13:o:5152:VAL:HG13 | 1.98                     | 0.63              |
| 18:y:5042:ARG:HB3  | 18:y:5043:ARG:HE   | 1.64                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:52:PHE:O       | 1:A:71:LEU:HD12    | 1.98                     | 0.63              |
| 1:A:192:ILE:HG12   | 1:A:293:MET:SD     | 2.37                     | 0.63              |
| 2:B:55:MET:HE3     | 2:B:80:ILE:HG21    | 1.78                     | 0.63              |
| 2:B:75:TRP:HE1     | 2:B:94:GLU:HB2     | 1.63                     | 0.63              |
| 2:B:451:PHE:HZ     | 22:B:1012:CLA:O1D  | 1.81                     | 0.63              |
| 22:C:1033:CLA:HHC  | 22:C:1033:CLA:CBB  | 2.27                     | 0.63              |
| 4:D:201:VAL:O      | 4:D:205:LEU:HB3    | 1.97                     | 0.63              |
| 5:E:17:VAL:O       | 5:E:21:VAL:HG23    | 1.98                     | 0.63              |
| 7:H:30:LEU:C       | 7:H:33:VAL:HG22    | 2.24                     | 0.63              |
| 8:I:4:LEU:O        | 8:I:8:VAL:HG22     | 1.97                     | 0.63              |
| 13:O:129:PHE:O     | 13:O:129:PHE:CD2   | 2.50                     | 0.63              |
| 13:O:152:VAL:O     | 13:O:152:VAL:HG13  | 1.98                     | 0.63              |
| 1:a:5105:TRP:HZ3   | 25:a:6044:BCR:H393 | 1.63                     | 0.63              |
| 3:c:5263:ALA:CB    | 3:c:5264:PHE:HD2   | 2.10                     | 0.63              |
| 3:c:5443:TRP:HA    | 3:c:5443:TRP:CE3   | 2.33                     | 0.63              |
| 15:u:5028:ASN:HD21 | 15:u:5055:TYR:N    | 1.95                     | 0.63              |
| 15:u:5053:ALA:HB1  | 15:u:5054:PRO:HD2  | 1.79                     | 0.63              |
| 18:y:5043:ARG:HH21 | 18:y:5044:GLY:CA   | 2.11                     | 0.63              |
| 18:y:5043:ARG:HD3  | 20:z:5031:GLN:HE21 | 1.63                     | 0.63              |
| 1:A:119:PHE:C      | 1:A:119:PHE:CD2    | 2.76                     | 0.63              |
| 22:A:1006:CLA:O2D  | 22:A:1006:CLA:H2A  | 1.99                     | 0.63              |
| 2:B:30:VAL:CG1     | 22:B:1013:CLA:HMD1 | 2.28                     | 0.63              |
| 22:B:1022:CLA:H121 | 12:M:24:ILE:HD12   | 1.80                     | 0.63              |
| 4:D:155:SER:HA     | 4:D:159:ILE:HB     | 1.78                     | 0.63              |
| 4:D:328:TRP:CZ3    | 16:V:161:VAL:HA    | 2.33                     | 0.63              |
| 11:L:29:LEU:HD13   | 11:L:29:LEU:O      | 1.98                     | 0.63              |
| 22:a:6006:CLA:HHC  | 22:a:6006:CLA:CBB  | 2.23                     | 0.63              |
| 2:b:5025:MET:C     | 2:b:5027:THR:H     | 2.06                     | 0.63              |
| 2:b:5452:THR:O     | 2:b:5456:ALA:HB2   | 1.99                     | 0.63              |
| 22:b:6018:CLA:H2A  | 22:b:6018:CLA:O2D  | 1.99                     | 0.63              |
| 3:c:5407:VAL:HG13  | 3:c:5407:VAL:O     | 1.99                     | 0.63              |
| 11:l:5026:VAL:HG12 | 11:l:5027:LEU:N    | 2.14                     | 0.63              |
| 1:A:325:ASN:ND2    | 1:A:328:MET:HE3    | 2.13                     | 0.63              |
| 2:B:97:ALA:C       | 2:B:99:ALA:N       | 2.54                     | 0.63              |
| 22:B:1014:CLA:C9   | 25:B:1048:BCR:H342 | 2.28                     | 0.63              |
| 3:C:425:TRP:CH2    | 22:C:1028:CLA:O1A  | 2.52                     | 0.63              |
| 22:C:1029:CLA:HMD2 | 22:C:1031:CLA:CAB  | 2.28                     | 0.63              |
| 22:C:1036:CLA:HBB1 | 22:C:1036:CLA:CHC  | 2.28                     | 0.63              |
| 4:D:87:HIS:NE2     | 4:D:162:LEU:HA     | 2.13                     | 0.63              |
| 4:D:123:ILE:O      | 4:D:127:LEU:HG     | 1.97                     | 0.63              |
| 13:O:104:LEU:HD12  | 13:O:104:LEU:O     | 1.98                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:Y:39:LEU:HD21   | 20:Z:28:ALA:CB     | 2.27                     | 0.63              |
| 2:b:5463:PHE:HE1   | 22:b:6016:CLA:CBB  | 2.12                     | 0.63              |
| 22:b:6011:CLA:H11  | 22:b:6011:CLA:CHB  | 2.29                     | 0.63              |
| 22:c:6030:CLA:HED3 | 22:c:6030:CLA:CHA  | 2.27                     | 0.63              |
| 24:d:6042:PQ9:H241 | 28:l:6061:MGE:H263 | 1.79                     | 0.63              |
| 7:h:5030:LEU:C     | 7:h:5033:VAL:HG22  | 2.24                     | 0.63              |
| 22:k:6034:CLA:O1D  | 22:k:6034:CLA:CAA  | 2.30                     | 0.63              |
| 15:u:5068:THR:HG22 | 15:u:5071:GLN:CB   | 2.28                     | 0.63              |
| 1:A:323:ARG:NE     | 4:D:332:GLN:NE2    | 2.46                     | 0.63              |
| 1:A:331:MET:HE1    | 4:D:348:ARG:CA     | 2.29                     | 0.63              |
| 2:B:103:LEU:HD12   | 2:B:107:LEU:HG     | 1.79                     | 0.63              |
| 2:B:357:ARG:HG2    | 2:B:357:ARG:NH1    | 2.08                     | 0.63              |
| 28:B:1060:MGE:CGB  | 28:B:1060:MGE:H211 | 2.29                     | 0.63              |
| 3:C:362:ARG:HD2    | 3:C:367:GLU:OE2    | 1.98                     | 0.63              |
| 3:C:417:VAL:CG1    | 16:V:68:VAL:HG11   | 2.25                     | 0.63              |
| 4:D:194:ASN:O      | 4:D:198:MET:HG3    | 1.97                     | 0.63              |
| 22:K:1034:CLA:H12  | 22:K:1034:CLA:ND   | 2.12                     | 0.63              |
| 12:M:9:ILE:CD1     | 12:m:5009:ILE:HD12 | 2.18                     | 0.63              |
| 20:Z:5:PHE:HE1     | 20:Z:54:VAL:HG13   | 1.63                     | 0.63              |
| 1:a:5338:ASN:O     | 1:a:5339:PHE:CG    | 2.51                     | 0.63              |
| 26:a:6063:LHG:HC82 | 3:c:5036:TRP:CE2   | 2.33                     | 0.63              |
| 3:c:5223:TRP:CD1   | 3:c:5224:ILE:CG1   | 2.81                     | 0.63              |
| 3:c:5280:SER:OG    | 3:c:5438:LEU:HB2   | 1.98                     | 0.63              |
| 22:h:6017:CLA:HBB1 | 25:h:6049:BCR:H322 | 1.79                     | 0.63              |
| 10:k:5033:PHE:O    | 10:k:5036:ALA:HB3  | 1.98                     | 0.63              |
| 1:A:254:TYR:CD2    | 4:D:132:ILE:HG22   | 2.34                     | 0.63              |
| 2:B:220:ARG:HG3    | 7:H:21:VAL:HA      | 1.80                     | 0.63              |
| 3:C:230:LEU:O      | 3:C:234:VAL:HG12   | 1.98                     | 0.63              |
| 3:C:418:ASN:OD1    | 29:C:1056:DGD:HE2  | 1.99                     | 0.63              |
| 3:C:437:PHE:HA     | 22:C:1032:CLA:HMC1 | 1.79                     | 0.63              |
| 3:C:443:TRP:CE3    | 3:C:443:TRP:HA     | 2.33                     | 0.63              |
| 22:C:1031:CLA:H2A  | 22:C:1031:CLA:O2D  | 1.98                     | 0.63              |
| 22:C:1032:CLA:HBC2 | 22:C:1032:CLA:HHD  | 1.79                     | 0.63              |
| 22:C:1032:CLA:H161 | 29:C:1056:DGD:CDB  | 2.29                     | 0.63              |
| 25:C:1054:BCR:C8   | 25:C:1054:BCR:H311 | 2.29                     | 0.63              |
| 22:K:1034:CLA:CGD  | 22:K:1034:CLA:CGA  | 2.76                     | 0.63              |
| 13:O:148:VAL:O     | 13:O:148:VAL:HG22  | 1.98                     | 0.63              |
| 18:Y:42:ARG:HB3    | 18:Y:43:ARG:HE     | 1.64                     | 0.63              |
| 1:a:5087:ASN:ND2   | 3:c:5357:ARG:HE    | 1.97                     | 0.63              |
| 1:a:5093:PHE:O     | 1:a:5095:PRO:HD3   | 1.99                     | 0.63              |
| 1:a:5105:TRP:CZ2   | 1:a:5111:PRO:HA    | 2.34                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:b:6060:MGE:CBB  | 28:b:6060:MGE:H263 | 2.28                     | 0.63              |
| 3:c:5042:LEU:CD1   | 3:c:5049:LEU:HD11  | 2.28                     | 0.63              |
| 3:c:5193:GLY:O     | 3:c:5194:GLY:C     | 2.40                     | 0.63              |
| 6:f:5021:VAL:O     | 6:f:5025:THR:HG23  | 1.98                     | 0.63              |
| 22:k:6034:CLA:CGD  | 22:k:6034:CLA:CGA  | 2.77                     | 0.63              |
| 1:A:93:PHE:O       | 1:A:95:PRO:HD3     | 1.99                     | 0.63              |
| 3:C:155:ASN:CA     | 3:C:158:THR:HG22   | 2.26                     | 0.63              |
| 3:C:170:ILE:HG22   | 3:C:171:GLY:N      | 2.13                     | 0.63              |
| 3:C:193:GLY:O      | 3:C:194:GLY:C      | 2.40                     | 0.63              |
| 3:C:223:TRP:CD1    | 3:C:224:ILE:CG1    | 2.81                     | 0.63              |
| 3:C:240:ILE:HG13   | 22:C:1025:CLA:CAB  | 2.29                     | 0.63              |
| 4:D:182:LEU:O      | 4:D:185:PHE:N      | 2.29                     | 0.63              |
| 4:D:189:HIS:CG     | 4:D:289:LEU:HD22   | 2.34                     | 0.63              |
| 22:D:1004:CLA:H142 | 22:D:1004:CLA:C10  | 2.28                     | 0.63              |
| 22:K:1034:CLA:C4D  | 22:K:1034:CLA:C1   | 2.77                     | 0.63              |
| 1:a:5012:ASN:O     | 1:a:5015:GLU:HG3   | 1.99                     | 0.63              |
| 1:a:5290:ILE:HG22  | 1:a:5291:SER:N     | 2.14                     | 0.63              |
| 22:a:6006:CLA:O2D  | 22:a:6006:CLA:H2A  | 1.99                     | 0.63              |
| 2:b:5103:LEU:HD13  | 22:b:6014:CLA:C9   | 2.28                     | 0.63              |
| 2:b:5249:ALA:O     | 2:b:5252:VAL:N     | 2.31                     | 0.63              |
| 2:b:5288:VAL:O     | 2:b:5292:LEU:HB2   | 1.99                     | 0.63              |
| 22:b:6011:CLA:CGA  | 22:b:6011:CLA:H42  | 2.28                     | 0.63              |
| 3:c:5223:TRP:HE1   | 3:c:5224:ILE:HG12  | 1.62                     | 0.63              |
| 3:c:5240:ILE:HG13  | 22:c:6025:CLA:CAB  | 2.29                     | 0.63              |
| 22:d:6005:CLA:H152 | 22:d:6005:CLA:H202 | 1.79                     | 0.63              |
| 10:k:5021:LEU:HD11 | 18:y:5024:MET:CG   | 2.27                     | 0.63              |
| 15:u:5016:LYS:HG2  | 15:u:5021:TYR:CD1  | 2.34                     | 0.63              |
| 15:u:5070:ARG:O    | 15:u:5073:GLN:HB3  | 1.99                     | 0.63              |
| 1:A:116:ILE:CD1    | 1:A:158:PHE:HB3    | 2.27                     | 0.63              |
| 2:B:111:ALA:C      | 2:B:113:TRP:H      | 2.07                     | 0.63              |
| 2:B:288:VAL:O      | 2:B:292:LEU:HB2    | 1.99                     | 0.63              |
| 3:C:280:SER:OG     | 3:C:438:LEU:HB2    | 1.98                     | 0.63              |
| 3:C:443:TRP:HA     | 3:C:443:TRP:HE3    | 1.64                     | 0.63              |
| 4:D:19:ASP:OD2     | 4:D:23:LYS:HD3     | 1.99                     | 0.63              |
| 5:E:47:PHE:C       | 5:E:49:THR:H       | 2.07                     | 0.63              |
| 25:H:1049:BCR:H401 | 17:X:20:PHE:HZ     | 1.64                     | 0.63              |
| 13:O:144:LEU:H     | 13:O:144:LEU:HD23  | 1.64                     | 0.63              |
| 15:U:70:ARG:O      | 15:U:73:GLN:HB3    | 1.99                     | 0.63              |
| 15:U:78:ASN:HB3    | 15:U:82:PHE:HE2    | 1.64                     | 0.63              |
| 16:V:38:LEU:O      | 16:V:94:ASN:HB3    | 1.99                     | 0.63              |
| 16:V:62:ALA:HB1    | 31:V:1041:HEM:HBB1 | 1.80                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5150:PRO:HA    | 22:a:6003:CLA:H52  | 1.81                     | 0.63              |
| 22:b:6009:CLA:C3D  | 22:b:6010:CLA:HBB2 | 2.26                     | 0.63              |
| 3:c:5229:ASN:H     | 3:c:5229:ASN:ND2   | 1.85                     | 0.63              |
| 3:c:5333:GLY:H     | 3:c:5338:GLY:CA    | 2.10                     | 0.63              |
| 4:d:5037:LEU:HD13  | 4:d:5125:PHE:HA    | 1.81                     | 0.63              |
| 5:e:5047:PHE:C     | 5:e:5049:THR:H     | 2.07                     | 0.63              |
| 22:k:6034:CLA:H12  | 22:k:6034:CLA:ND   | 2.12                     | 0.63              |
| 15:u:5078:ASN:HB3  | 15:u:5082:PHE:HE2  | 1.64                     | 0.63              |
| 1:A:105:TRP:HZ3    | 25:A:1044:BCR:H393 | 1.62                     | 0.63              |
| 1:A:212:CYS:CB     | 4:D:211:CYS:HB2    | 2.24                     | 0.63              |
| 22:A:1006:CLA:C17  | 25:D:1050:BCR:C27  | 2.66                     | 0.63              |
| 22:A:1007:CLA:H71  | 22:A:1007:CLA:H41  | 1.80                     | 0.63              |
| 24:A:1043:PQ9:H293 | 23:D:1039:PHO:CBA  | 2.29                     | 0.63              |
| 2:B:63:LEU:N       | 2:B:64:PRO:CD      | 2.61                     | 0.63              |
| 3:C:146:PHE:O      | 3:C:146:PHE:CD1    | 2.52                     | 0.63              |
| 3:C:159:THR:HA     | 3:C:252:ILE:HA     | 1.81                     | 0.63              |
| 23:D:1039:PHO:CMA  | 22:D:1004:CLA:H102 | 2.28                     | 0.63              |
| 8:I:9:TYR:O        | 8:I:12:VAL:HG12    | 1.99                     | 0.63              |
| 1:a:5196:PRO:HB2   | 29:c:6057:DGD:C8A  | 2.26                     | 0.63              |
| 2:b:5297:THR:OG1   | 2:b:5300:GLU:HG3   | 1.99                     | 0.63              |
| 2:b:5372:ASP:HB3   | 2:b:5376:VAL:HB    | 1.79                     | 0.63              |
| 3:c:5049:LEU:HD22  | 3:c:5052:ALA:CA    | 2.29                     | 0.63              |
| 22:c:6035:CLA:H2A  | 22:c:6035:CLA:O2D  | 1.99                     | 0.63              |
| 29:c:6055:DGD:HAT1 | 29:c:6055:DGD:HA61 | 1.78                     | 0.63              |
| 4:d:5106:GLN:C     | 4:d:5108:GLY:H     | 2.07                     | 0.63              |
| 4:d:5145:ALA:HB2   | 4:d:5272:LEU:CD1   | 2.28                     | 0.63              |
| 4:d:5189:HIS:CG    | 4:d:5289:LEU:HD22  | 2.34                     | 0.63              |
| 1:A:335:ASN:ND2    | 13:O:182:PHE:CE1   | 2.67                     | 0.62              |
| 26:A:1063:LHG:HC82 | 3:C:36:TRP:CE2     | 2.33                     | 0.62              |
| 2:B:15:ASP:N       | 2:B:16:PRO:HD3     | 2.14                     | 0.62              |
| 3:C:51:GLY:O       | 3:C:55:ALA:N       | 2.24                     | 0.62              |
| 3:C:184:GLY:O      | 3:C:185:LEU:HD23   | 1.99                     | 0.62              |
| 3:C:265:ILE:CD1    | 3:C:452:ALA:CB     | 2.61                     | 0.62              |
| 11:L:26:VAL:HG12   | 11:L:27:LEU:N      | 2.14                     | 0.62              |
| 25:T:6048:BCR:C34  | 22:b:6023:CLA:H41  | 2.29                     | 0.62              |
| 18:Y:43:ARG:HH21   | 18:Y:44:GLY:CA     | 2.12                     | 0.62              |
| 2:b:5111:ALA:C     | 2:b:5113:TRP:H     | 2.07                     | 0.62              |
| 3:c:5171:GLY:HA3   | 22:c:6025:CLA:HBC1 | 1.81                     | 0.62              |
| 3:c:5377:LEU:C     | 3:c:5377:LEU:HD13  | 2.24                     | 0.62              |
| 3:c:5417:VAL:HG12  | 16:v:5068:VAL:CB   | 2.21                     | 0.62              |
| 3:c:5418:ASN:OD1   | 29:c:6056:DGD:HE2  | 1.99                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5061:HIS:HE1   | 4:d:5080:THR:HG23  | 1.63                     | 0.62              |
| 4:d:5279:LEU:HD21  | 23:d:6039:PHO:HMC1 | 1.80                     | 0.62              |
| 22:d:6005:CLA:C12  | 22:d:6005:CLA:H92  | 2.28                     | 0.62              |
| 15:u:5016:LYS:HZ1  | 15:u:5085:THR:HB   | 1.64                     | 0.62              |
| 23:A:1038:PHO:HHD  | 23:A:1038:PHO:CBC  | 2.28                     | 0.62              |
| 22:C:1035:CLA:O2D  | 22:C:1035:CLA:H2A  | 1.99                     | 0.62              |
| 4:D:150:ILE:O      | 4:D:154:VAL:HG23   | 1.99                     | 0.62              |
| 25:D:1050:BCR:C22  | 28:D:1059:MGE:C3A  | 2.75                     | 0.62              |
| 16:V:119:PRO:HA    | 16:V:127:PHE:CD2   | 2.35                     | 0.62              |
| 1:a:5322:ASN:HA    | 1:a:5325:ASN:HB2   | 1.82                     | 0.62              |
| 2:b:5178:VAL:O     | 2:b:5178:VAL:HG13  | 1.98                     | 0.62              |
| 2:b:5220:ARG:HG3   | 7:h:5021:VAL:HA    | 1.80                     | 0.62              |
| 2:b:5271:THR:HG23  | 2:b:5274:GLN:HB2   | 1.81                     | 0.62              |
| 3:c:5039:ASN:HB2   | 22:c:6032:CLA:CBA  | 2.28                     | 0.62              |
| 3:c:5362:ARG:HD2   | 3:c:5367:GLU:OE2   | 1.98                     | 0.62              |
| 4:d:5273:PHE:O     | 4:d:5274:VAL:C     | 2.42                     | 0.62              |
| 4:d:5328:TRP:CZ3   | 16:v:5161:VAL:HA   | 2.33                     | 0.62              |
| 25:d:6050:BCR:C22  | 28:d:6059:MGE:C3A  | 2.75                     | 0.62              |
| 8:i:5005:LYS:O     | 8:i:5008:VAL:HG23  | 2.00                     | 0.62              |
| 8:i:5009:TYR:O     | 8:i:5012:VAL:HG12  | 1.99                     | 0.62              |
| 13:o:5068:ARG:O    | 13:o:5068:ARG:HG3  | 2.00                     | 0.62              |
| 15:u:5045:LEU:HD13 | 15:u:5071:GLN:HG2  | 1.80                     | 0.62              |
| 1:A:87:ASN:ND2     | 3:C:357:ARG:HE     | 1.97                     | 0.62              |
| 1:A:309:ALA:HB3    | 16:V:28:GLU:HB2    | 1.79                     | 0.62              |
| 22:B:1011:CLA:CAA  | 22:B:1011:CLA:CGD  | 2.77                     | 0.62              |
| 22:B:1011:CLA:H11  | 22:B:1011:CLA:CHB  | 2.29                     | 0.62              |
| 6:F:21:VAL:O       | 6:F:25:THR:HG23    | 1.98                     | 0.62              |
| 1:a:5059:ASP:O     | 1:a:5060:ILE:C     | 2.42                     | 0.62              |
| 1:a:5254:TYR:CD2   | 4:d:5132:ILE:HG22  | 2.34                     | 0.62              |
| 22:a:6006:CLA:HBC2 | 4:d:5182:LEU:HD21  | 1.81                     | 0.62              |
| 22:a:6007:CLA:O1D  | 22:a:6007:CLA:H2A  | 1.98                     | 0.62              |
| 22:b:6013:CLA:HMC1 | 22:b:6013:CLA:HBC3 | 1.81                     | 0.62              |
| 3:c:5165:LEU:HB2   | 3:c:5248:GLY:CA    | 2.29                     | 0.62              |
| 4:d:5087:HIS:NE2   | 4:d:5162:LEU:HA    | 2.13                     | 0.62              |
| 4:d:5184:PHE:CE2   | 4:d:5188:PHE:HD1   | 2.11                     | 0.62              |
| 25:k:6051:BCR:H353 | 18:y:5032:GLY:CA   | 2.20                     | 0.62              |
| 13:o:5144:LEU:HD23 | 13:o:5144:LEU:H    | 1.64                     | 0.62              |
| 16:v:5062:ALA:HB1  | 31:v:6041:HEM:HBB1 | 1.80                     | 0.62              |
| 1:A:105:TRP:CZ2    | 1:A:111:PRO:HA     | 2.34                     | 0.62              |
| 1:A:223:LEU:HD21   | 4:D:265:ARG:CG     | 2.29                     | 0.62              |
| 24:A:1043:PQ9:H37  | 24:A:1043:PQ9:C29  | 2.29                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:45:PHE:HA      | 2:B:58:GLN:HE22    | 1.64                     | 0.62              |
| 2:B:103:LEU:HD13   | 22:B:1014:CLA:C9   | 2.28                     | 0.62              |
| 2:B:452:THR:O      | 2:B:456:ALA:HB2    | 1.99                     | 0.62              |
| 25:B:1048:BCR:H371 | 25:B:1048:BCR:H392 | 1.32                     | 0.62              |
| 3:C:58:GLY:HA2     | 3:C:61:VAL:HG12    | 1.82                     | 0.62              |
| 3:C:318:LEU:HD23   | 3:C:318:LEU:O      | 1.98                     | 0.62              |
| 22:C:1035:CLA:H141 | 25:K:1051:BCR:C34  | 2.30                     | 0.62              |
| 4:D:174:GLY:HA3    | 4:D:177:ALA:HB3    | 1.81                     | 0.62              |
| 8:I:5:LYS:O        | 8:I:8:VAL:HG23     | 2.00                     | 0.62              |
| 11:L:20:GLY:HA3    | 12:M:22:LEU:HD13   | 1.82                     | 0.62              |
| 1:a:5199:GLN:O     | 1:a:5202:VAL:HG12  | 1.98                     | 0.62              |
| 1:a:5336:ALA:O     | 1:a:5337:HIS:C     | 2.42                     | 0.62              |
| 22:a:6007:CLA:H112 | 22:a:6007:CLA:C5   | 2.30                     | 0.62              |
| 2:b:5181:VAL:CG1   | 2:b:5196:GLY:HA2   | 2.29                     | 0.62              |
| 22:b:6018:CLA:H141 | 22:b:6018:CLA:H172 | 1.82                     | 0.62              |
| 22:b:6023:CLA:H152 | 22:b:6024:CLA:C4A  | 2.30                     | 0.62              |
| 3:c:5351:PHE:CD2   | 3:c:5375:LEU:HD11  | 2.34                     | 0.62              |
| 10:k:5020:PRO:HA   | 18:y:5021:GLN:HG2  | 1.81                     | 0.62              |
| 11:l:5020:GLY:HA3  | 12:m:5022:LEU:HD13 | 1.82                     | 0.62              |
| 16:v:5038:LEU:O    | 16:v:5094:ASN:HB3  | 1.99                     | 0.62              |
| 1:A:41:LEU:HD22    | 1:A:41:LEU:N       | 2.15                     | 0.62              |
| 1:A:199:GLN:O      | 1:A:202:VAL:HG12   | 1.98                     | 0.62              |
| 2:B:134:ASP:O      | 2:B:138:MET:HE2    | 2.00                     | 0.62              |
| 2:B:138:MET:SD     | 22:B:1023:CLA:HAC2 | 2.40                     | 0.62              |
| 22:B:1018:CLA:O2D  | 22:B:1018:CLA:H2A  | 1.99                     | 0.62              |
| 3:C:48:LYS:CD      | 22:C:1035:CLA:HED1 | 2.27                     | 0.62              |
| 3:C:165:LEU:HB2    | 3:C:248:GLY:CA     | 2.30                     | 0.62              |
| 22:C:1033:CLA:HMA3 | 22:K:1034:CLA:HMC2 | 1.81                     | 0.62              |
| 4:D:106:GLN:C      | 4:D:108:GLY:H      | 2.07                     | 0.62              |
| 4:D:170:ALA:O      | 4:D:171:PRO:O      | 2.18                     | 0.62              |
| 23:D:1039:PHO:HMA3 | 22:D:1004:CLA:H142 | 1.76                     | 0.62              |
| 8:I:13:THR:O       | 8:I:14:PHE:C       | 2.43                     | 0.62              |
| 10:K:20:PRO:HA     | 18:Y:21:GLN:HG2    | 1.81                     | 0.62              |
| 1:a:5215:HIS:CD2   | 1:a:5275:LEU:HD11  | 2.35                     | 0.62              |
| 2:b:5121:GLU:CB    | 7:h:5004:ARG:HB3   | 2.29                     | 0.62              |
| 2:b:5225:LEU:HD11  | 7:h:5028:THR:OG1   | 2.00                     | 0.62              |
| 3:c:5293:ASN:ND2   | 3:c:5295:THR:HB    | 2.15                     | 0.62              |
| 3:c:5437:PHE:HA    | 22:c:6032:CLA:HMC1 | 1.79                     | 0.62              |
| 3:c:5438:LEU:HD13  | 3:c:5438:LEU:C     | 2.24                     | 0.62              |
| 22:c:6035:CLA:HBB2 | 22:k:6034:CLA:CHB  | 2.29                     | 0.62              |
| 22:c:6036:CLA:HBB1 | 22:c:6036:CLA:CHC  | 2.28                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5078:VAL:HG12  | 4:d:5173:PHE:HB3   | 1.82                     | 0.62              |
| 25:d:6050:BCR:C38  | 25:d:6050:BCR:C23  | 2.59                     | 0.62              |
| 16:v:5105:PRO:HG2  | 16:v:5115:ALA:N    | 2.14                     | 0.62              |
| 2:B:24:LEU:HD21    | 2:B:110:ALA:O      | 1.99                     | 0.62              |
| 2:B:24:LEU:HD23    | 2:B:111:ALA:HA     | 1.81                     | 0.62              |
| 2:B:112:CYS:SG     | 14:t:5023:PHE:CZ   | 2.91                     | 0.62              |
| 28:B:1060:MGE:H5B2 | 4:D:276:VAL:HB     | 1.81                     | 0.62              |
| 3:C:75:PHE:CD1     | 3:C:86:LEU:HD11    | 2.34                     | 0.62              |
| 22:C:1028:CLA:HMC2 | 22:K:1034:CLA:HED1 | 1.81                     | 0.62              |
| 4:D:275:PRO:O      | 4:D:277:THR:N      | 2.33                     | 0.62              |
| 28:D:1059:MGE:O5D  | 6:F:40:MET:HB2     | 2.00                     | 0.62              |
| 28:D:1062:MGE:O1A  | 28:D:1062:MGE:H4B1 | 2.00                     | 0.62              |
| 25:H:1049:BCR:H321 | 25:H:1049:BCR:C8   | 2.29                     | 0.62              |
| 8:I:16:VAL:O       | 8:I:20:VAL:HG23    | 2.00                     | 0.62              |
| 13:O:181:ASN:O     | 13:O:182:PHE:HB2   | 1.99                     | 0.62              |
| 15:U:16:LYS:HG2    | 15:U:21:TYR:CD1    | 2.34                     | 0.62              |
| 16:V:105:PRO:HG2   | 16:V:115:ALA:N     | 2.14                     | 0.62              |
| 24:a:6043:PQ9:H37  | 24:a:6043:PQ9:C30  | 2.29                     | 0.62              |
| 24:a:6043:PQ9:H293 | 23:d:6039:PHO:CBA  | 2.29                     | 0.62              |
| 22:b:6011:CLA:O1A  | 22:b:6011:CLA:H42  | 1.98                     | 0.62              |
| 3:c:5425:TRP:CH2   | 22:c:6028:CLA:O1A  | 2.52                     | 0.62              |
| 22:c:6025:CLA:O2A  | 22:c:6025:CLA:H3A  | 1.99                     | 0.62              |
| 22:c:6030:CLA:HMB2 | 22:c:6031:CLA:C4B  | 2.07                     | 0.62              |
| 5:e:5013:ILE:HG13  | 5:e:5019:TYR:HB2   | 1.79                     | 0.62              |
| 6:f:5045:ARG:HE    | 6:f:5045:ARG:CA    | 1.97                     | 0.62              |
| 14:t:5018:PHE:CD1  | 25:t:1046:BCR:H332 | 2.33                     | 0.62              |
| 20:z:5005:PHE:HE1  | 20:z:5054:VAL:HG13 | 1.63                     | 0.62              |
| 2:B:91:TRP:CD1     | 22:B:1014:CLA:HBA2 | 2.35                     | 0.62              |
| 2:B:297:THR:OG1    | 2:B:300:GLU:HG3    | 1.99                     | 0.62              |
| 22:B:1014:CLA:CBC  | 22:B:1014:CLA:CHD  | 2.72                     | 0.62              |
| 3:C:386:PRO:HB2    | 16:V:116:GLU:OE1   | 2.00                     | 0.62              |
| 4:D:274:VAL:HG22   | 24:D:1042:PQ9:H261 | 1.81                     | 0.62              |
| 16:V:54:GLU:OE2    | 16:V:57:ARG:HD3    | 1.99                     | 0.62              |
| 1:a:5223:LEU:O     | 1:a:5224:ILE:CB    | 2.41                     | 0.62              |
| 24:a:6043:PQ9:H37  | 24:a:6043:PQ9:C29  | 2.30                     | 0.62              |
| 2:b:5091:TRP:CD1   | 22:b:6014:CLA:HBA2 | 2.35                     | 0.62              |
| 3:c:5184:GLY:O     | 3:c:5185:LEU:HD23  | 1.99                     | 0.62              |
| 3:c:5230:LEU:O     | 3:c:5234:VAL:HG12  | 1.98                     | 0.62              |
| 22:c:6029:CLA:H51  | 22:c:6029:CLA:NB   | 2.15                     | 0.62              |
| 22:c:6035:CLA:C3B  | 25:k:6052:BCR:H271 | 2.29                     | 0.62              |
| 25:c:6054:BCR:C8   | 25:c:6054:BCR:H311 | 2.29                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:h:6049:BCR:H401 | 17:x:5020:PHE:HZ   | 1.64                     | 0.62              |
| 8:i:5016:VAL:O     | 8:i:5020:VAL:HG23  | 2.00                     | 0.62              |
| 22:k:6034:CLA:C4D  | 22:k:6034:CLA:C1   | 2.77                     | 0.62              |
| 1:A:160:ILE:HD13   | 3:C:431:PHE:CE1    | 2.35                     | 0.62              |
| 1:A:215:HIS:CD2    | 1:A:275:LEU:HD11   | 2.35                     | 0.62              |
| 1:A:290:ILE:HG22   | 1:A:291:SER:N      | 2.14                     | 0.62              |
| 2:B:23:HIS:O       | 2:B:27:THR:HB      | 1.98                     | 0.62              |
| 2:B:24:LEU:HD21    | 2:B:110:ALA:C      | 2.25                     | 0.62              |
| 2:B:25:MET:C       | 2:B:27:THR:H       | 2.06                     | 0.62              |
| 2:B:181:VAL:CG1    | 2:B:196:GLY:HA2    | 2.29                     | 0.62              |
| 2:B:315:ILE:HG22   | 2:B:426:PHE:O      | 1.99                     | 0.62              |
| 22:B:1013:CLA:HBC3 | 22:B:1013:CLA:HMC1 | 1.81                     | 0.62              |
| 22:B:1023:CLA:C9   | 22:B:1024:CLA:H152 | 2.30                     | 0.62              |
| 3:C:407:VAL:O      | 3:C:407:VAL:HG13   | 1.99                     | 0.62              |
| 22:C:1035:CLA:HBB2 | 22:K:1034:CLA:CHB  | 2.29                     | 0.62              |
| 6:F:34:LEU:HD12    | 9:J:24:ILE:CD1     | 2.28                     | 0.62              |
| 2:b:5024:LEU:HD21  | 2:b:5110:ALA:O     | 1.99                     | 0.62              |
| 3:c:5146:PHE:O     | 3:c:5146:PHE:CD1   | 2.52                     | 0.62              |
| 3:c:5160:ILE:HG22  | 3:c:5161:LEU:N     | 2.14                     | 0.62              |
| 4:d:5019:ASP:OD2   | 4:d:5023:LYS:HD3   | 1.99                     | 0.62              |
| 4:d:5054:PHE:HB3   | 5:e:5047:PHE:HD1   | 1.65                     | 0.62              |
| 7:h:5012:ARG:N     | 7:h:5013:PRO:HD2   | 2.15                     | 0.62              |
| 15:u:5043:PRO:HG3  | 16:v:5108:TYR:C    | 2.25                     | 0.62              |
| 16:v:5119:PRO:HA   | 16:v:5127:PHE:CD2  | 2.34                     | 0.62              |
| 18:y:5043:ARG:CD   | 18:y:5044:GLY:N    | 2.63                     | 0.62              |
| 1:A:270:SER:O      | 1:A:273:PHE:HB3    | 2.00                     | 0.62              |
| 3:C:135:ARG:HG2    | 20:Z:27:TYR:HB3    | 1.82                     | 0.62              |
| 22:C:1025:CLA:C9   | 25:C:1054:BCR:H373 | 2.29                     | 0.62              |
| 22:C:1035:CLA:C3B  | 25:C:1052:BCR:H271 | 2.29                     | 0.62              |
| 4:D:61:HIS:HE1     | 4:D:80:THR:HG23    | 1.63                     | 0.62              |
| 4:D:223:PHE:CE1    | 4:D:245:SER:HB2    | 2.35                     | 0.62              |
| 5:E:77:GLU:O       | 5:E:81:GLU:N       | 2.33                     | 0.62              |
| 15:U:45:LEU:HD13   | 15:U:71:GLN:HG2    | 1.80                     | 0.62              |
| 1:a:5052:PHE:O     | 1:a:5071:LEU:HD12  | 1.98                     | 0.62              |
| 1:a:5331:MET:HE1   | 4:d:5348:ARG:CA    | 2.29                     | 0.62              |
| 2:b:5002:GLY:C     | 11:l:5011:GLU:HB2  | 2.25                     | 0.62              |
| 2:b:5134:ASP:O     | 2:b:5138:MET:HE2   | 2.00                     | 0.62              |
| 2:b:5315:ILE:HG22  | 2:b:5426:PHE:O     | 1.99                     | 0.62              |
| 22:b:6015:CLA:H91  | 22:b:6015:CLA:H122 | 1.80                     | 0.62              |
| 3:c:5117:VAL:HG21  | 22:c:6027:CLA:H162 | 1.81                     | 0.62              |
| 4:d:5150:ILE:O     | 4:d:5154:VAL:HG23  | 1.99                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:v:5094:ASN:C    | 16:v:5096:GLU:N    | 2.52                     | 0.62              |
| 1:A:330:VAL:HG11   | 4:D:348:ARG:HG2    | 1.82                     | 0.62              |
| 2:B:2:GLY:C        | 11:L:11:GLU:HB2    | 2.25                     | 0.62              |
| 2:B:121:GLU:CB     | 7:H:4:ARG:HB3      | 2.29                     | 0.62              |
| 2:B:225:LEU:HD11   | 7:H:28:THR:OG1     | 2.00                     | 0.62              |
| 2:B:419:SER:HA     | 2:B:422:ARG:HH12   | 1.65                     | 0.62              |
| 3:C:438:LEU:HD13   | 3:C:438:LEU:C      | 2.24                     | 0.62              |
| 3:C:451:ALA:CA     | 3:C:456:GLU:HG2    | 2.30                     | 0.62              |
| 11:L:22:LEU:HG     | 28:L:1061:MGE:H221 | 1.82                     | 0.62              |
| 13:O:59:ASP:H      | 13:O:64:TYR:HE1    | 1.47                     | 0.62              |
| 14:T:8:PHE:CE1     | 27:T:1066:IOD:I    | 3.23                     | 0.62              |
| 1:a:5064:ARG:NH2   | 13:o:5131:PRO:O    | 2.33                     | 0.62              |
| 1:a:5320:ILE:O     | 1:a:5321:ILE:C     | 2.43                     | 0.62              |
| 1:a:5335:ASN:ND2   | 13:o:5182:PHE:CE1  | 2.67                     | 0.62              |
| 2:b:5138:MET:SD    | 22:b:6023:CLA:HAC2 | 2.40                     | 0.62              |
| 22:b:6023:CLA:C15  | 22:b:6024:CLA:C4A  | 2.78                     | 0.62              |
| 3:c:5216:SER:HB2   | 3:c:5221:GLU:HB2   | 1.82                     | 0.62              |
| 3:c:5275:SER:CB    | 22:c:6033:CLA:HED1 | 2.20                     | 0.62              |
| 3:c:5348:GLU:HB3   | 13:o:5042:ALA:HB3  | 1.79                     | 0.62              |
| 4:d:5036:LEU:HD23  | 4:d:5037:LEU:H     | 1.65                     | 0.62              |
| 4:d:5219:GLU:O     | 4:d:5222:LEU:HB2   | 2.00                     | 0.62              |
| 4:d:5274:VAL:HG22  | 24:d:6042:PQ9:H261 | 1.82                     | 0.62              |
| 23:d:6039:PHO:CMA  | 22:d:6004:CLA:H102 | 2.28                     | 0.62              |
| 28:d:6059:MGE:CBB  | 28:d:6059:MGE:CFB  | 2.47                     | 0.62              |
| 5:e:5077:GLU:O     | 5:e:5081:GLU:N     | 2.33                     | 0.62              |
| 6:f:5040:MET:HB3   | 6:f:5043:ILE:HD11  | 1.82                     | 0.62              |
| 7:h:5030:LEU:HB3   | 22:h:6017:CLA:CMD  | 2.30                     | 0.62              |
| 13:o:5148:VAL:O    | 13:o:5148:VAL:HG22 | 1.98                     | 0.62              |
| 15:u:5059:GLU:C    | 15:u:5061:VAL:N    | 2.58                     | 0.62              |
| 16:v:5054:GLU:OE2  | 16:v:5057:ARG:HD3  | 1.99                     | 0.62              |
| 1:A:64:ARG:NH2     | 13:O:131:PRO:O     | 2.33                     | 0.61              |
| 22:A:1007:CLA:H112 | 22:A:1007:CLA:C5   | 2.30                     | 0.61              |
| 2:B:222:PRO:HB2    | 2:B:225:LEU:HD13   | 1.82                     | 0.61              |
| 2:B:271:THR:HG23   | 2:B:274:GLN:HB2    | 1.81                     | 0.61              |
| 2:B:285:ASN:HA     | 2:B:288:VAL:HG12   | 1.82                     | 0.61              |
| 2:B:429:ILE:H      | 2:B:429:ILE:CD1    | 2.13                     | 0.61              |
| 22:B:1016:CLA:H162 | 22:D:1008:CLA:HMA1 | 0.64                     | 0.61              |
| 22:B:1019:CLA:HMD2 | 28:B:1060:MGE:C1G  | 2.29                     | 0.61              |
| 22:B:1023:CLA:H41  | 25:B:1048:BCR:C34  | 2.29                     | 0.61              |
| 3:C:42:LEU:HD13    | 3:C:49:LEU:HD11    | 1.80                     | 0.61              |
| 3:C:321:ASP:O      | 3:C:324:LEU:N      | 2.33                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:327:ASN:HD21   | 3:C:330:SER:C      | 2.08                     | 0.61              |
| 3:C:377:LEU:C      | 3:C:377:LEU:HD13   | 2.24                     | 0.61              |
| 22:C:1033:CLA:HMA1 | 22:K:1034:CLA:C3C  | 2.25                     | 0.61              |
| 22:D:1008:CLA:C19  | 22:D:1008:CLA:H141 | 2.18                     | 0.61              |
| 7:H:30:LEU:HB3     | 22:H:1017:CLA:CMD  | 2.30                     | 0.61              |
| 16:V:66:CYS:SG     | 31:V:1041:HEM:C3C  | 2.93                     | 0.61              |
| 1:a:5126:TYR:C     | 1:a:5126:TYR:CD2   | 2.76                     | 0.61              |
| 1:a:5290:ILE:CG2   | 1:a:5291:SER:N     | 2.63                     | 0.61              |
| 2:b:5090:PHE:HZ    | 2:b:5098:LEU:HD12  | 1.65                     | 0.61              |
| 2:b:5133:LEU:HA    | 7:h:5015:ASN:HD21  | 1.65                     | 0.61              |
| 28:b:6060:MGE:H5B2 | 4:d:5276:VAL:HB    | 1.81                     | 0.61              |
| 3:c:5240:ILE:O     | 3:c:5240:ILE:HD13  | 2.00                     | 0.61              |
| 22:c:6028:CLA:C9   | 29:c:6056:DGD:HB91 | 2.30                     | 0.61              |
| 25:c:6054:BCR:H23C | 25:c:6054:BCR:H402 | 1.73                     | 0.61              |
| 29:c:6056:DGD:HB1  | 29:c:6056:DGD:CAB  | 2.30                     | 0.61              |
| 4:d:5275:PRO:O     | 4:d:5277:THR:N     | 2.33                     | 0.61              |
| 22:d:6005:CLA:H93  | 28:d:6062:MGE:H211 | 1.82                     | 0.61              |
| 22:d:6004:CLA:H142 | 22:d:6004:CLA:C10  | 2.28                     | 0.61              |
| 22:d:6008:CLA:HMA2 | 22:d:6008:CLA:CBA  | 2.02                     | 0.61              |
| 5:e:5011:SER:O     | 5:e:5015:THR:HB    | 2.00                     | 0.61              |
| 1:A:297:LEU:CD2    | 3:C:404:LEU:HD23   | 2.30                     | 0.61              |
| 1:A:322:ASN:HA     | 1:A:325:ASN:HB2    | 1.82                     | 0.61              |
| 22:A:1006:CLA:HHC  | 22:A:1006:CLA:CBB  | 2.23                     | 0.61              |
| 2:B:90:PHE:HZ      | 2:B:98:LEU:HD12    | 1.65                     | 0.61              |
| 3:C:39:ASN:HB2     | 22:C:1032:CLA:CBA  | 2.28                     | 0.61              |
| 3:C:160:ILE:HG22   | 3:C:161:LEU:N      | 2.14                     | 0.61              |
| 3:C:264:PHE:O      | 3:C:266:TRP:CD1    | 2.54                     | 0.61              |
| 13:O:92:VAL:HG13   | 13:O:93:PRO:HD2    | 1.83                     | 0.61              |
| 13:O:251:MET:H     | 13:O:251:MET:HE2   | 1.65                     | 0.61              |
| 15:U:43:PRO:HG3    | 16:V:108:TYR:C     | 2.25                     | 0.61              |
| 2:b:5017:GLY:HA2   | 2:b:5123:PHE:CE1   | 2.35                     | 0.61              |
| 2:b:5024:LEU:HD23  | 2:b:5111:ALA:HA    | 1.81                     | 0.61              |
| 3:c:5048:LYS:CD    | 22:c:6035:CLA:HED1 | 2.27                     | 0.61              |
| 23:d:6039:PHO:O2D  | 23:d:6039:PHO:H2A  | 2.01                     | 0.61              |
| 13:o:5181:ASN:O    | 13:o:5182:PHE:HB2  | 1.99                     | 0.61              |
| 16:v:5066:CYS:SG   | 31:v:6041:HEM:C3C  | 2.94                     | 0.61              |
| 1:A:59:ASP:O       | 1:A:60:ILE:C       | 2.43                     | 0.61              |
| 1:A:273:PHE:CE1    | 26:A:1063:LHG:HC61 | 2.35                     | 0.61              |
| 1:A:320:ILE:O      | 1:A:321:ILE:C      | 2.43                     | 0.61              |
| 22:B:1023:CLA:H152 | 22:B:1024:CLA:C4A  | 2.29                     | 0.61              |
| 3:C:49:LEU:HD22    | 3:C:52:ALA:CA      | 2.29                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:351:PHE:CD2    | 3:C:375:LEU:HD11   | 2.35                     | 0.61              |
| 22:C:1028:CLA:C6   | 29:C:1057:DGD:HA42 | 2.31                     | 0.61              |
| 4:D:54:PHE:HB3     | 5:E:47:PHE:HD1     | 1.65                     | 0.61              |
| 5:E:11:SER:O       | 5:E:15:THR:HB      | 2.00                     | 0.61              |
| 1:a:5160:ILE:HD13  | 3:c:5431:PHE:CE1   | 2.35                     | 0.61              |
| 1:a:5273:PHE:CE1   | 26:a:6063:LHG:HC61 | 2.35                     | 0.61              |
| 1:a:5340:PRO:HD3   | 15:u:5103:TYR:CE2  | 2.36                     | 0.61              |
| 23:a:6038:PHO:HHD  | 23:a:6038:PHO:CBC  | 2.28                     | 0.61              |
| 2:b:5135:LEU:HD12  | 2:b:5135:LEU:N     | 2.15                     | 0.61              |
| 22:b:6011:CLA:HAA1 | 22:b:6011:CLA:CGD  | 2.30                     | 0.61              |
| 22:b:6016:CLA:H162 | 22:d:6008:CLA:HMA1 | 0.64                     | 0.61              |
| 3:c:5386:PRO:HB2   | 16:v:5116:GLU:OE1  | 2.00                     | 0.61              |
| 3:c:5443:TRP:HA    | 3:c:5443:TRP:HE3   | 1.64                     | 0.61              |
| 8:i:5029:ALA:O     | 8:i:5030:ARG:HB2   | 2.01                     | 0.61              |
| 13:o:5251:MET:H    | 13:o:5251:MET:HE2  | 1.65                     | 0.61              |
| 16:v:5038:LEU:CA   | 16:v:5045:ILE:HD11 | 2.31                     | 0.61              |
| 16:v:5062:ALA:O    | 16:v:5063:CYS:CB   | 2.48                     | 0.61              |
| 1:A:197:PHE:HD1    | 1:A:285:PHE:HB3    | 1.65                     | 0.61              |
| 1:A:300:PHE:HB3    | 1:A:302:PHE:CE1    | 2.36                     | 0.61              |
| 2:B:135:LEU:HD12   | 2:B:135:LEU:N      | 2.15                     | 0.61              |
| 22:B:1023:CLA:C15  | 22:B:1024:CLA:C4A  | 2.78                     | 0.61              |
| 3:C:117:VAL:HG11   | 22:C:1027:CLA:C1   | 2.31                     | 0.61              |
| 22:C:1033:CLA:HMA3 | 22:K:1034:CLA:C2C  | 2.30                     | 0.61              |
| 25:C:1052:BCR:H361 | 10:K:32:PHE:HE2    | 1.63                     | 0.61              |
| 12:M:3:VAL:HG23    | 12:M:4:ASN:O       | 2.01                     | 0.61              |
| 15:U:27:LEU:HD21   | 15:U:82:PHE:HD1    | 1.65                     | 0.61              |
| 1:a:5041:LEU:HD22  | 1:a:5041:LEU:N     | 2.15                     | 0.61              |
| 1:a:5171:GLY:O     | 1:a:5172:MET:C     | 2.44                     | 0.61              |
| 2:b:5451:PHE:HZ    | 22:b:6012:CLA:O1D  | 1.81                     | 0.61              |
| 22:c:6029:CLA:HMD2 | 22:c:6031:CLA:CAB  | 2.28                     | 0.61              |
| 29:c:6056:DGD:HB81 | 29:c:6056:DGD:HBV2 | 1.81                     | 0.61              |
| 4:d:5313:THR:O     | 4:d:5316:THR:HG23  | 2.00                     | 0.61              |
| 28:d:6059:MGE:O5D  | 6:f:5040:MET:HB2   | 2.00                     | 0.61              |
| 8:i:5004:LEU:HA    | 8:i:5007:THR:OG1   | 2.00                     | 0.61              |
| 12:m:5003:VAL:HG23 | 12:m:5004:ASN:O    | 2.01                     | 0.61              |
| 13:o:5188:ARG:CB   | 13:o:5188:ARG:HH11 | 2.14                     | 0.61              |
| 13:o:5206:GLU:O    | 13:o:5207:GLU:CB   | 2.49                     | 0.61              |
| 16:v:5066:CYS:O    | 16:v:5073:LYS:CG   | 2.49                     | 0.61              |
| 1:A:340:PRO:HD3    | 15:U:103:TYR:CE2   | 2.36                     | 0.61              |
| 22:A:1003:CLA:CED  | 22:A:1003:CLA:C2A  | 2.64                     | 0.61              |
| 24:A:1043:PQ9:H37  | 24:A:1043:PQ9:C30  | 2.29                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:17:GLY:HA2     | 2:B:123:PHE:CE1    | 2.35                     | 0.61              |
| 2:B:99:ALA:HB1     | 22:B:1014:CLA:H43  | 1.82                     | 0.61              |
| 2:B:463:PHE:HE1    | 22:B:1016:CLA:CBB  | 2.12                     | 0.61              |
| 22:B:1019:CLA:HBB2 | 22:B:1021:CLA:HMB3 | 1.82                     | 0.61              |
| 3:C:240:ILE:HD13   | 3:C:240:ILE:O      | 2.00                     | 0.61              |
| 3:C:363:GLY:O      | 3:C:367:GLU:HG2    | 2.00                     | 0.61              |
| 25:C:1052:BCR:H352 | 25:K:1051:BCR:H322 | 1.82                     | 0.61              |
| 29:C:1056:DGD:HB81 | 29:C:1056:DGD:HBV2 | 1.81                     | 0.61              |
| 13:O:132:VAL:CG2   | 13:O:144:LEU:HD21  | 2.30                     | 0.61              |
| 13:O:188:ARG:CB    | 13:O:188:ARG:HH11  | 2.14                     | 0.61              |
| 16:V:151:ILE:HG12  | 16:V:152:LEU:N     | 2.15                     | 0.61              |
| 1:a:5267:ASN:HB3   | 1:a:5270:SER:HG    | 1.64                     | 0.61              |
| 1:a:5300:PHE:HB3   | 1:a:5302:PHE:CE1   | 2.36                     | 0.61              |
| 2:b:5015:ASP:N     | 2:b:5016:PRO:HD3   | 2.14                     | 0.61              |
| 2:b:5024:LEU:HD21  | 2:b:5110:ALA:C     | 2.25                     | 0.61              |
| 22:b:6011:CLA:CGD  | 22:b:6011:CLA:CAA  | 2.77                     | 0.61              |
| 3:c:5117:VAL:HG11  | 22:c:6027:CLA:C1   | 2.31                     | 0.61              |
| 3:c:5135:ARG:HG2   | 20:z:5027:TYR:HB3  | 1.82                     | 0.61              |
| 3:c:5263:ALA:HB1   | 3:c:5264:PHE:CE2   | 2.34                     | 0.61              |
| 3:c:5451:ALA:CA    | 3:c:5456:GLU:HG2   | 2.30                     | 0.61              |
| 22:c:6028:CLA:O2A  | 29:c:6056:DGD:HG11 | 2.01                     | 0.61              |
| 22:c:6035:CLA:H141 | 25:k:6051:BCR:C34  | 2.30                     | 0.61              |
| 4:d:5264:LYS:O     | 4:d:5268:HIS:ND1   | 2.34                     | 0.61              |
| 6:f:5020:TRP:HE1   | 6:f:5024:HIS:CE1   | 2.18                     | 0.61              |
| 1:A:185:VAL:O      | 1:A:188:ALA:HB3    | 2.00                     | 0.61              |
| 1:A:290:ILE:CG2    | 1:A:291:SER:N      | 2.63                     | 0.61              |
| 22:C:1031:CLA:CBC  | 22:C:1031:CLA:CHD  | 2.71                     | 0.61              |
| 4:D:219:GLU:O      | 4:D:222:LEU:HB2    | 2.00                     | 0.61              |
| 22:D:1005:CLA:H93  | 28:D:1062:MGE:H211 | 1.83                     | 0.61              |
| 6:F:41:GLN:NE2     | 9:J:31:GLY:HA3     | 2.16                     | 0.61              |
| 7:H:12:ARG:N       | 7:H:13:PRO:HD2     | 2.15                     | 0.61              |
| 13:O:68:ARG:HG3    | 13:O:68:ARG:O      | 2.00                     | 0.61              |
| 16:V:38:LEU:HA     | 16:V:95:ILE:CG2    | 2.26                     | 0.61              |
| 20:Z:20:VAL:O      | 20:Z:24:PRO:CD     | 2.45                     | 0.61              |
| 2:b:5374:ASN:HD22  | 2:b:5374:ASN:N     | 1.98                     | 0.61              |
| 22:b:6014:CLA:CBC  | 22:b:6014:CLA:CHD  | 2.72                     | 0.61              |
| 22:b:6023:CLA:C9   | 22:b:6024:CLA:H152 | 2.30                     | 0.61              |
| 3:c:5159:THR:HA    | 3:c:5252:ILE:HA    | 1.81                     | 0.61              |
| 22:c:6028:CLA:C6   | 29:c:6057:DGD:HA42 | 2.31                     | 0.61              |
| 22:c:6028:CLA:HMC2 | 22:k:6034:CLA:HED1 | 1.81                     | 0.61              |
| 29:c:6056:DGD:HB51 | 9:j:5029:PHE:HE1   | 1.66                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5059:ASP:H    | 13:o:5064:TYR:HE1  | 1.47                     | 0.61              |
| 29:C:1056:DGD:HB51 | 9:J:29:PHE:HE1     | 1.66                     | 0.61              |
| 1:a:5272:HIS:O     | 4:d:5215:GLY:CA    | 2.48                     | 0.61              |
| 1:a:5317:TRP:HA    | 4:d:5063:LEU:HD11  | 1.83                     | 0.61              |
| 1:a:5325:ASN:ND2   | 1:a:5328:MET:HE3   | 2.13                     | 0.61              |
| 22:a:6007:CLA:H71  | 22:a:6007:CLA:H41  | 1.81                     | 0.61              |
| 2:b:5468:TRP:CE3   | 4:d:5144:ILE:HD13  | 2.36                     | 0.61              |
| 22:b:6011:CLA:CMD  | 22:b:6014:CLA:CMB  | 2.79                     | 0.61              |
| 28:b:6060:MGE:CGB  | 28:b:6060:MGE:H211 | 2.29                     | 0.61              |
| 3:c:5264:PHE:O     | 3:c:5266:TRP:CD1   | 2.54                     | 0.61              |
| 22:c:6029:CLA:C1A  | 22:c:6029:CLA:CGA  | 2.78                     | 0.61              |
| 22:c:6036:CLA:HHC  | 22:c:6036:CLA:CBB  | 2.29                     | 0.61              |
| 4:d:5173:PHE:CD1   | 23:d:6039:PHO:H13  | 2.36                     | 0.61              |
| 4:d:5174:GLY:HA3   | 4:d:5177:ALA:HB3   | 1.81                     | 0.61              |
| 4:d:5223:PHE:CE1   | 4:d:5245:SER:HB2   | 2.35                     | 0.61              |
| 1:A:12:ASN:O       | 1:A:15:GLU:HG3     | 1.99                     | 0.61              |
| 1:A:171:GLY:O      | 1:A:172:MET:C      | 2.44                     | 0.61              |
| 22:A:1007:CLA:H112 | 22:A:1007:CLA:C6   | 2.29                     | 0.61              |
| 24:A:1043:PQ9:C45  | 28:D:1059:MGE:C9A  | 2.79                     | 0.61              |
| 2:B:174:LEU:HD21   | 2:B:312:TYR:HE1    | 1.66                     | 0.61              |
| 3:C:293:ASN:ND2    | 3:C:295:THR:HB     | 2.15                     | 0.61              |
| 4:D:190:ASN:HD22   | 4:D:296:TYR:HA     | 1.66                     | 0.61              |
| 4:D:313:THR:O      | 4:D:316:THR:HG23   | 2.00                     | 0.61              |
| 25:K:1051:BCR:H353 | 18:Y:32:GLY:CA     | 2.20                     | 0.61              |
| 16:V:39:ASN:C      | 16:V:41:GLU:H      | 2.09                     | 0.61              |
| 2:b:5099:ALA:HB1   | 22:b:6014:CLA:H43  | 1.82                     | 0.61              |
| 2:b:5113:TRP:CD1   | 2:b:5114:HIS:N     | 2.69                     | 0.61              |
| 3:c:5274:TYR:O     | 3:c:5276:LEU:N     | 2.34                     | 0.61              |
| 3:c:5327:ASN:HD21  | 3:c:5330:SER:C     | 2.08                     | 0.61              |
| 3:c:5384:ILE:O     | 3:c:5384:ILE:HG23  | 2.00                     | 0.61              |
| 22:c:6026:CLA:C7   | 22:c:6026:CLA:C12  | 2.76                     | 0.61              |
| 4:d:5210:LEU:HD11  | 24:d:6042:PQ9:H152 | 1.82                     | 0.61              |
| 28:d:6062:MGE:O1A  | 28:d:6062:MGE:H4B1 | 2.00                     | 0.61              |
| 13:o:5148:VAL:HG23 | 13:o:5172:PHE:HE2  | 1.66                     | 0.61              |
| 22:A:1007:CLA:H41  | 22:A:1007:CLA:C7   | 2.30                     | 0.61              |
| 22:B:1011:CLA:CGD  | 22:B:1011:CLA:HAA1 | 2.30                     | 0.61              |
| 22:B:1011:CLA:C1D  | 22:B:1013:CLA:C3   | 2.78                     | 0.61              |
| 22:C:1030:CLA:CBC  | 22:C:1030:CLA:CHD  | 2.58                     | 0.61              |
| 4:D:37:LEU:HD13    | 4:D:125:PHE:HA     | 1.81                     | 0.61              |
| 4:D:210:LEU:HD11   | 24:D:1042:PQ9:H152 | 1.82                     | 0.61              |
| 8:I:29:ALA:O       | 8:I:30:ARG:HB2     | 2.01                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:O:223:ILE:HD13  | 13:O:225:LEU:HD13  | 1.83                     | 0.61              |
| 1:a:5217:SER:O     | 1:a:5220:THR:HG22  | 2.01                     | 0.61              |
| 1:a:5315:ASN:O     | 4:d:5063:LEU:HD23  | 2.01                     | 0.61              |
| 1:a:5331:MET:HE1   | 4:d:5348:ARG:N     | 2.16                     | 0.61              |
| 22:a:6007:CLA:H41  | 22:a:6007:CLA:C7   | 2.30                     | 0.61              |
| 22:b:6009:CLA:CGA  | 22:b:6009:CLA:NA   | 2.64                     | 0.61              |
| 22:b:6011:CLA:O2D  | 22:b:6012:CLA:HED1 | 2.00                     | 0.61              |
| 29:b:6058:DGD:CAB  | 29:b:6058:DGD:HB62 | 2.31                     | 0.61              |
| 4:d:5035:ILE:O     | 4:d:5039:PRO:HG3   | 2.01                     | 0.61              |
| 4:d:5190:ASN:HD22  | 4:d:5296:TYR:HA    | 1.66                     | 0.61              |
| 7:h:5043:LEU:HD23  | 7:h:5043:LEU:C     | 2.26                     | 0.61              |
| 18:y:5045:ASN:C    | 18:y:5045:ASN:ND2  | 2.59                     | 0.61              |
| 2:B:113:TRP:CD1    | 2:B:114:HIS:N      | 2.69                     | 0.61              |
| 2:B:133:LEU:HA     | 7:H:15:ASN:HD21    | 1.65                     | 0.61              |
| 22:B:1018:CLA:H141 | 22:B:1018:CLA:H172 | 1.82                     | 0.61              |
| 3:C:117:VAL:HG21   | 22:C:1027:CLA:H162 | 1.81                     | 0.61              |
| 3:C:171:GLY:HA3    | 22:C:1025:CLA:HBC1 | 1.81                     | 0.61              |
| 22:C:1025:CLA:O2A  | 22:C:1025:CLA:H3A  | 1.99                     | 0.61              |
| 22:C:1026:CLA:C7   | 22:C:1026:CLA:C12  | 2.76                     | 0.61              |
| 6:F:20:TRP:HE1     | 6:F:24:HIS:CE1     | 2.18                     | 0.61              |
| 7:H:43:LEU:HD23    | 7:H:43:LEU:C       | 2.26                     | 0.61              |
| 9:J:15:THR:HG21    | 10:K:38:VAL:HG22   | 1.82                     | 0.61              |
| 13:O:55:ALA:CB     | 13:O:161:SER:HB3   | 2.30                     | 0.61              |
| 1:a:5142:TRP:HB3   | 3:c:5443:TRP:CZ2   | 2.36                     | 0.61              |
| 1:a:5172:MET:HE2   | 1:a:5179:THR:CB    | 2.31                     | 0.61              |
| 2:b:5124:ARG:HE    | 2:b:5131:PRO:HB3   | 1.66                     | 0.61              |
| 22:b:6011:CLA:CMD  | 22:b:6014:CLA:HMB2 | 2.31                     | 0.61              |
| 22:b:6019:CLA:HBB2 | 22:b:6021:CLA:HMB3 | 1.82                     | 0.61              |
| 3:c:5089:ILE:HA    | 3:c:5092:ILE:HD13  | 1.83                     | 0.61              |
| 3:c:5264:PHE:O     | 3:c:5266:TRP:NE1   | 2.34                     | 0.61              |
| 3:c:5363:GLY:O     | 3:c:5367:GLU:HG2   | 2.00                     | 0.61              |
| 22:c:6025:CLA:C4   | 22:c:6025:CLA:C1B  | 2.77                     | 0.61              |
| 22:c:6033:CLA:HHC  | 22:c:6033:CLA:CBB  | 2.27                     | 0.61              |
| 22:c:6033:CLA:HMA3 | 22:k:6034:CLA:HMC2 | 1.81                     | 0.61              |
| 29:c:6057:DGD:HG31 | 9:j:5033:TYR:CE2   | 2.35                     | 0.61              |
| 25:h:6049:BCR:H321 | 25:h:6049:BCR:C8   | 2.29                     | 0.61              |
| 16:v:5094:ASN:HB2  | 16:v:5097:GLY:H    | 1.66                     | 0.61              |
| 16:v:5105:PRO:HG3  | 16:v:5115:ALA:HA   | 1.83                     | 0.61              |
| 16:v:5151:ILE:HG12 | 16:v:5152:LEU:N    | 2.15                     | 0.61              |
| 20:z:5027:TYR:H    | 20:z:5027:TYR:HD2  | 1.49                     | 0.61              |
| 1:A:331:MET:HE1    | 4:D:348:ARG:N      | 2.16                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1028:CLA:C9   | 29:C:1056:DGD:HB91 | 2.30                     | 0.60              |
| 4:D:78:VAL:HG12    | 4:D:173:PHE:HB3    | 1.82                     | 0.60              |
| 4:D:282:SER:C      | 22:D:1004:CLA:CED  | 2.74                     | 0.60              |
| 23:D:1039:PHO:H2A  | 23:D:1039:PHO:O2D  | 2.01                     | 0.60              |
| 25:H:1049:BCR:C23  | 25:H:1049:BCR:H393 | 2.30                     | 0.60              |
| 1:a:5151:LEU:HG    | 1:a:5155:PHE:HD2   | 1.65                     | 0.60              |
| 1:a:5270:SER:O     | 1:a:5273:PHE:HB3   | 2.00                     | 0.60              |
| 1:a:5331:MET:O     | 1:a:5332:HIS:C     | 2.44                     | 0.60              |
| 2:b:5045:PHE:HA    | 2:b:5058:GLN:HE22  | 1.64                     | 0.60              |
| 4:d:5058:TRP:C     | 4:d:5058:TRP:CD1   | 2.79                     | 0.60              |
| 1:A:142:TRP:HB3    | 3:C:443:TRP:CZ2    | 2.36                     | 0.60              |
| 1:A:151:LEU:HG     | 1:A:155:PHE:HD2    | 1.65                     | 0.60              |
| 1:A:197:PHE:CE2    | 29:C:1056:DGD:HAN2 | 2.37                     | 0.60              |
| 2:B:49:ASP:OD1     | 2:B:53:ASN:N       | 2.34                     | 0.60              |
| 3:C:223:TRP:CD1    | 3:C:224:ILE:N      | 2.69                     | 0.60              |
| 3:C:318:LEU:HD23   | 3:C:328:VAL:HG11   | 1.83                     | 0.60              |
| 29:C:1057:DGD:HG31 | 9:J:33:TYR:CE2     | 2.35                     | 0.60              |
| 4:D:221:THR:HG21   | 4:D:245:SER:O      | 2.01                     | 0.60              |
| 11:L:9:PRO:HG2     | 12:m:5034:LYS:HG3  | 1.83                     | 0.60              |
| 13:O:62:GLN:HA     | 13:O:62:GLN:HE21   | 1.66                     | 0.60              |
| 1:a:5193:LEU:HD22  | 4:d:5179:PHE:CD2   | 2.36                     | 0.60              |
| 1:a:5297:LEU:CD2   | 3:c:5404:LEU:HD23  | 2.29                     | 0.60              |
| 1:a:5334:ARG:HB2   | 1:a:5335:ASN:OD1   | 2.02                     | 0.60              |
| 2:b:5222:PRO:HB2   | 2:b:5225:LEU:HD13  | 1.82                     | 0.60              |
| 22:b:6011:CLA:C1D  | 22:b:6013:CLA:C3   | 2.78                     | 0.60              |
| 3:c:5075:PHE:CD1   | 3:c:5086:LEU:HD11  | 2.34                     | 0.60              |
| 3:c:5155:ASN:CA    | 3:c:5158:THR:HG22  | 2.26                     | 0.60              |
| 22:c:6026:CLA:CGA  | 22:c:6026:CLA:H42  | 2.31                     | 0.60              |
| 4:d:5183:LEU:HD23  | 4:d:5183:LEU:N     | 2.14                     | 0.60              |
| 13:o:5062:GLN:HA   | 13:o:5062:GLN:HE21 | 1.66                     | 0.60              |
| 13:o:5083:LYS:HD2  | 13:o:5085:LYS:HE3  | 1.83                     | 0.60              |
| 13:o:5092:VAL:HG13 | 13:o:5093:PRO:HD2  | 1.83                     | 0.60              |
| 1:A:129:ARG:O      | 1:A:129:ARG:HG2    | 2.01                     | 0.60              |
| 22:A:1006:CLA:HBC2 | 4:D:182:LEU:HD21   | 1.81                     | 0.60              |
| 22:B:1011:CLA:CMD  | 22:B:1014:CLA:HMB2 | 2.31                     | 0.60              |
| 3:C:263:ALA:HB1    | 3:C:264:PHE:CE2    | 2.34                     | 0.60              |
| 22:C:1035:CLA:CMD  | 10:K:40:GLN:NE2    | 2.64                     | 0.60              |
| 4:D:39:PRO:O       | 4:D:43:LEU:HG      | 2.01                     | 0.60              |
| 8:I:4:LEU:HA       | 8:I:7:THR:OG1      | 2.00                     | 0.60              |
| 13:O:66:ILE:HD12   | 13:O:121:PHE:CD1   | 2.36                     | 0.60              |
| 13:O:82:PRO:HG3    | 13:O:89:ALA:CB     | 2.31                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5063:ILE:HG12  | 1:a:5064:ARG:N     | 2.15                     | 0.60              |
| 1:a:5185:VAL:O     | 1:a:5188:ALA:HB3   | 2.00                     | 0.60              |
| 22:a:6007:CLA:CAD  | 22:a:6007:CLA:CED  | 2.80                     | 0.60              |
| 3:c:5056:HIS:C     | 3:c:5056:HIS:HD2   | 2.07                     | 0.60              |
| 3:c:5436:PHE:O     | 3:c:5439:VAL:HB    | 2.00                     | 0.60              |
| 4:d:5297:ASP:CG    | 4:d:5298:PHE:N     | 2.60                     | 0.60              |
| 1:A:140:ARG:NH1    | 1:A:140:ARG:CB     | 2.64                     | 0.60              |
| 1:A:217:SER:O      | 1:A:220:THR:HG22   | 2.01                     | 0.60              |
| 2:B:62:VAL:CG1     | 22:B:1013:CLA:HED2 | 2.31                     | 0.60              |
| 22:B:1011:CLA:CMD  | 22:B:1014:CLA:CMB  | 2.79                     | 0.60              |
| 22:B:1011:CLA:O2D  | 22:B:1012:CLA:HED1 | 2.00                     | 0.60              |
| 29:B:1058:DGD:CAB  | 29:B:1058:DGD:HB62 | 2.31                     | 0.60              |
| 3:C:216:SER:HB2    | 3:C:221:GLU:HB2    | 1.82                     | 0.60              |
| 3:C:384:ILE:HG23   | 3:C:384:ILE:O      | 2.00                     | 0.60              |
| 22:C:1028:CLA:O2A  | 29:C:1056:DGD:HG11 | 2.00                     | 0.60              |
| 22:C:1029:CLA:CGA  | 22:C:1029:CLA:C1A  | 2.78                     | 0.60              |
| 4:D:325:ILE:O      | 4:D:329:MET:HG2    | 2.02                     | 0.60              |
| 6:F:41:GLN:HE21    | 9:J:28:PHE:HA      | 1.65                     | 0.60              |
| 16:V:66:CYS:O      | 16:V:73:LYS:CG     | 2.49                     | 0.60              |
| 1:a:5119:PHE:CD2   | 1:a:5123:ALA:HB2   | 2.36                     | 0.60              |
| 1:a:5136:ARG:HH12  | 8:i:5027:ASP:HB3   | 1.67                     | 0.60              |
| 1:a:5140:ARG:NH1   | 1:a:5140:ARG:CB    | 2.64                     | 0.60              |
| 1:a:5142:TRP:HZ2   | 4:d:5219:GLU:HG3   | 1.67                     | 0.60              |
| 1:a:5190:HIS:HE1   | 1:a:5296:ASN:HD22  | 1.50                     | 0.60              |
| 1:a:5197:PHE:HD1   | 1:a:5285:PHE:HB3   | 1.66                     | 0.60              |
| 2:b:5006:TYR:OH    | 28:l:6061:MGE:H2D  | 2.01                     | 0.60              |
| 2:b:5062:VAL:CG1   | 22:b:6013:CLA:HED2 | 2.31                     | 0.60              |
| 2:b:5174:LEU:HD21  | 2:b:5312:TYR:HE1   | 1.66                     | 0.60              |
| 22:b:6022:CLA:H91  | 22:b:6022:CLA:C12  | 1.92                     | 0.60              |
| 3:c:5223:TRP:CD1   | 3:c:5224:ILE:N     | 2.69                     | 0.60              |
| 3:c:5321:ASP:O     | 3:c:5324:LEU:N     | 2.33                     | 0.60              |
| 22:c:6035:CLA:C2B  | 25:k:6052:BCR:C27  | 2.77                     | 0.60              |
| 29:c:6055:DGD:HB21 | 29:c:6055:DGD:C2A  | 2.30                     | 0.60              |
| 4:d:5282:SER:C     | 22:d:6004:CLA:CED  | 2.74                     | 0.60              |
| 6:f:5037:ILE:HA    | 6:f:5040:MET:HE3   | 1.82                     | 0.60              |
| 14:t:5021:ILE:HD12 | 25:t:1046:BCR:HC42 | 1.84                     | 0.60              |
| 1:A:256:GLY:HA2    | 1:A:264:SER:HB2    | 1.84                     | 0.60              |
| 1:A:315:ASN:O      | 4:D:63:LEU:HD23    | 2.01                     | 0.60              |
| 1:A:336:ALA:O      | 1:A:338:ASN:ND2    | 2.34                     | 0.60              |
| 2:B:111:ALA:O      | 2:B:113:TRP:N      | 2.34                     | 0.60              |
| 2:B:468:TRP:CE3    | 4:D:144:ILE:HD13   | 2.36                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1033:CLA:HBB1 | 22:C:1033:CLA:CHC  | 2.25                     | 0.60              |
| 4:D:313:THR:OG1    | 4:D:316:THR:HG22   | 2.01                     | 0.60              |
| 14:T:18:PHE:HD1    | 25:T:6046:BCR:H332 | 1.66                     | 0.60              |
| 16:V:94:ASN:HB2    | 16:V:97:GLY:H      | 1.66                     | 0.60              |
| 1:a:5151:LEU:HD21  | 29:c:6055:DGD:HBS2 | 1.83                     | 0.60              |
| 1:a:5197:PHE:CE2   | 29:c:6056:DGD:HAN2 | 2.37                     | 0.60              |
| 2:b:5055:MET:HE3   | 2:b:5080:ILE:CG2   | 2.32                     | 0.60              |
| 2:b:5111:ALA:O     | 2:b:5113:TRP:N     | 2.34                     | 0.60              |
| 2:b:5419:SER:HA    | 2:b:5422:ARG:HH12  | 1.65                     | 0.60              |
| 22:b:6021:CLA:H2   | 22:b:6021:CLA:HED1 | 1.79                     | 0.60              |
| 4:d:5022:LEU:O     | 4:d:5030:VAL:O     | 2.20                     | 0.60              |
| 13:o:5082:PRO:HG3  | 13:o:5089:ALA:CB   | 2.31                     | 0.60              |
| 1:A:172:MET:HE2    | 1:A:179:THR:CB     | 2.31                     | 0.60              |
| 1:A:219:VAL:HG21   | 4:D:268:HIS:CD2    | 2.36                     | 0.60              |
| 1:A:317:TRP:HA     | 4:D:63:LEU:HD11    | 1.83                     | 0.60              |
| 2:B:124:ARG:HE     | 2:B:131:PRO:HB3    | 1.66                     | 0.60              |
| 22:B:1022:CLA:H93  | 22:B:1022:CLA:C12  | 2.09                     | 0.60              |
| 3:C:271:TYR:HE1    | 22:C:1031:CLA:HAC1 | 1.64                     | 0.60              |
| 4:D:36:LEU:HD23    | 4:D:37:LEU:H       | 1.65                     | 0.60              |
| 4:D:103:ARG:HD2    | 5:E:76:VAL:HG21    | 1.84                     | 0.60              |
| 4:D:352:LEU:H      | 4:D:352:LEU:CD2    | 2.15                     | 0.60              |
| 16:V:38:LEU:CA     | 16:V:45:ILE:HD11   | 2.31                     | 0.60              |
| 1:a:5320:ILE:HG21  | 4:d:5180:ARG:HG3   | 1.84                     | 0.60              |
| 2:b:5075:TRP:HE1   | 2:b:5094:GLU:HB2   | 1.63                     | 0.60              |
| 2:b:5188:ASP:OD1   | 2:b:5191:ASN:HB2   | 2.02                     | 0.60              |
| 3:c:5171:GLY:HA2   | 3:c:5174:LEU:CB    | 2.22                     | 0.60              |
| 3:c:5431:PHE:C     | 3:c:5431:PHE:CD2   | 2.79                     | 0.60              |
| 22:c:6025:CLA:H171 | 22:c:6031:CLA:H102 | 1.84                     | 0.60              |
| 29:c:6055:DGD:CEB  | 29:c:6055:DGD:HBG3 | 2.25                     | 0.60              |
| 4:d:5039:PRO:O     | 4:d:5043:LEU:HG    | 2.01                     | 0.60              |
| 4:d:5251:ARG:HH22  | 4:d:5255:GLN:HE22  | 1.49                     | 0.60              |
| 11:l:5022:LEU:HG   | 28:l:6061:MGE:H221 | 1.82                     | 0.60              |
| 16:v:5039:ASN:C    | 16:v:5041:GLU:H    | 2.09                     | 0.60              |
| 1:A:193:LEU:HD22   | 4:D:179:PHE:CD2    | 2.36                     | 0.60              |
| 3:C:264:PHE:O      | 3:C:266:TRP:NE1    | 2.34                     | 0.60              |
| 3:C:436:PHE:O      | 3:C:439:VAL:HB     | 2.00                     | 0.60              |
| 4:D:22:LEU:O       | 4:D:30:VAL:O       | 2.20                     | 0.60              |
| 4:D:148:ALA:HB2    | 4:D:276:VAL:HG12   | 1.84                     | 0.60              |
| 4:D:273:PHE:O      | 4:D:274:VAL:C      | 2.42                     | 0.60              |
| 6:F:37:ILE:HA      | 6:F:40:MET:HE3     | 1.82                     | 0.60              |
| 13:O:90:GLU:OE1    | 13:O:90:GLU:HA     | 2.00                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:O:107:ILE:HG23  | 13:O:123:GLU:HG3   | 1.84                     | 0.60              |
| 13:O:206:GLU:O     | 13:O:207:GLU:CB    | 2.48                     | 0.60              |
| 15:U:31:ASN:ND2    | 15:U:32:ILE:N      | 2.48                     | 0.60              |
| 15:U:52:ASN:OD1    | 15:U:64:ILE:HD13   | 2.02                     | 0.60              |
| 20:Z:55:GLY:HA2    | 25:Z:1053:BCR:H313 | 1.82                     | 0.60              |
| 1:a:5187:GLN:HG3   | 1:a:5325:ASN:ND2   | 2.10                     | 0.60              |
| 2:b:5429:ILE:H     | 2:b:5429:ILE:CD1   | 2.13                     | 0.60              |
| 22:b:6020:CLA:H8   | 22:b:6020:CLA:H41  | 1.84                     | 0.60              |
| 4:d:5090:LEU:CD1   | 4:d:5096:GLU:HG3   | 2.31                     | 0.60              |
| 4:d:5170:ALA:O     | 4:d:5171:PRO:O     | 2.18                     | 0.60              |
| 4:d:5313:THR:OG1   | 4:d:5316:THR:HG22  | 2.01                     | 0.60              |
| 13:o:5072:GLN:HA   | 13:o:5103:SER:OG   | 2.02                     | 0.60              |
| 15:u:5068:THR:HG22 | 15:u:5071:GLN:N    | 2.10                     | 0.60              |
| 1:A:119:PHE:CD2    | 1:A:123:ALA:HB2    | 2.37                     | 0.60              |
| 1:A:258:LEU:O      | 1:A:259:ILE:HD12   | 2.01                     | 0.60              |
| 2:B:91:TRP:CG      | 22:B:1014:CLA:HBA2 | 2.37                     | 0.60              |
| 3:C:146:PHE:O      | 3:C:148:GLY:N      | 2.34                     | 0.60              |
| 3:C:274:TYR:O      | 3:C:276:LEU:N      | 2.34                     | 0.60              |
| 22:C:1029:CLA:C5   | 22:C:1029:CLA:C1C  | 2.79                     | 0.60              |
| 22:C:1037:CLA:HBB1 | 22:C:1037:CLA:CHC  | 2.14                     | 0.60              |
| 4:D:136:VAL:O      | 4:D:136:VAL:HG12   | 2.00                     | 0.60              |
| 6:F:40:MET:HB3     | 6:F:43:ILE:HD11    | 1.82                     | 0.60              |
| 20:Z:49:ALA:O      | 20:Z:53:VAL:HG23   | 2.01                     | 0.60              |
| 1:a:5223:LEU:HD21  | 4:d:5265:ARG:CG    | 2.29                     | 0.60              |
| 2:b:5049:ASP:OD1   | 2:b:5053:ASN:N     | 2.34                     | 0.60              |
| 3:c:5058:GLY:HA2   | 3:c:5061:VAL:HG12  | 1.82                     | 0.60              |
| 3:c:5087:ILE:HG22  | 3:c:5426:LEU:HD11  | 1.83                     | 0.60              |
| 22:c:6033:CLA:CMA  | 22:k:6034:CLA:CMC  | 2.80                     | 0.60              |
| 4:d:5136:VAL:HG12  | 4:d:5136:VAL:O     | 2.00                     | 0.60              |
| 25:k:6052:BCR:H352 | 25:k:6051:BCR:H322 | 1.82                     | 0.60              |
| 20:z:5027:TYR:HD2  | 20:z:5027:TYR:N    | 1.99                     | 0.60              |
| 1:A:14:TRP:CD1     | 1:A:14:TRP:C       | 2.80                     | 0.60              |
| 1:A:63:ILE:HG12    | 1:A:64:ARG:N       | 2.15                     | 0.60              |
| 1:A:136:ARG:HH12   | 8:I:27:ASP:HB3     | 1.67                     | 0.60              |
| 1:A:201:GLY:O      | 1:A:205:VAL:HG12   | 2.01                     | 0.60              |
| 22:A:1007:CLA:CAD  | 22:A:1007:CLA:CED  | 2.80                     | 0.60              |
| 23:A:1038:PHO:C9   | 22:D:1005:CLA:C18  | 2.80                     | 0.60              |
| 2:B:46:ASP:HB3     | 2:B:58:GLN:OE1     | 2.01                     | 0.60              |
| 2:B:374:ASN:HD22   | 2:B:374:ASN:N      | 1.98                     | 0.60              |
| 2:B:406:LEU:O      | 2:B:407:ASN:O      | 2.20                     | 0.60              |
| 22:B:1018:CLA:OBD  | 22:B:1018:CLA:C14  | 2.49                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:276:LEU:HD23   | 3:C:276:LEU:O      | 2.02                     | 0.60              |
| 3:C:279:LEU:O      | 3:C:280:SER:C      | 2.44                     | 0.60              |
| 3:C:431:PHE:C      | 3:C:431:PHE:CD2    | 2.79                     | 0.60              |
| 24:D:1042:PQ9:H292 | 24:D:1042:PQ9:H243 | 1.84                     | 0.60              |
| 20:Z:27:TYR:N      | 20:Z:27:TYR:HD2    | 1.99                     | 0.60              |
| 24:a:6043:PQ9:C45  | 28:d:6059:MGE:C9A  | 2.79                     | 0.60              |
| 2:b:5046:ASP:HB3   | 2:b:5058:GLN:OE1   | 2.01                     | 0.60              |
| 2:b:5170:ASP:CB    | 2:b:5171:PRO:HD2   | 2.32                     | 0.60              |
| 2:b:5285:ASN:HA    | 2:b:5288:VAL:HG12  | 1.82                     | 0.60              |
| 22:b:6021:CLA:HED3 | 22:b:6021:CLA:CGA  | 2.32                     | 0.60              |
| 4:d:5160:TYR:HB3   | 4:d:5161:PRO:HD3   | 1.83                     | 0.60              |
| 7:h:5055:LEU:HB2   | 7:h:5058:VAL:HB    | 1.83                     | 0.60              |
| 13:o:5066:ILE:HD12 | 13:o:5121:PHE:CD1  | 2.36                     | 0.60              |
| 1:A:147:TYR:C      | 1:A:150:PRO:HD2    | 2.27                     | 0.60              |
| 1:A:196:PRO:CA     | 1:A:199:GLN:HG3    | 2.31                     | 0.60              |
| 1:A:213:ALA:HB3    | 23:D:1039:PHO:HBC1 | 1.84                     | 0.60              |
| 2:B:15:ASP:CG      | 2:B:15:ASP:O       | 2.45                     | 0.60              |
| 22:B:1020:CLA:H8   | 22:B:1020:CLA:H41  | 1.84                     | 0.60              |
| 22:C:1029:CLA:HHC  | 22:C:1029:CLA:CBB  | 2.32                     | 0.60              |
| 4:D:58:TRP:CD1     | 4:D:58:TRP:C       | 2.79                     | 0.60              |
| 4:D:90:LEU:CD1     | 4:D:96:GLU:HG3     | 2.31                     | 0.60              |
| 4:D:219:GLU:OE1    | 4:D:219:GLU:HA     | 2.01                     | 0.60              |
| 1:a:5014:TRP:CD1   | 1:a:5014:TRP:C     | 2.80                     | 0.60              |
| 1:a:5244:GLU:HG2   | 4:d:5264:LYS:NZ    | 2.17                     | 0.60              |
| 22:a:6006:CLA:H91  | 22:d:6004:CLA:H171 | 1.84                     | 0.60              |
| 22:b:6011:CLA:C4D  | 22:b:6013:CLA:C2   | 2.80                     | 0.60              |
| 28:b:6060:MGE:H6D1 | 4:d:5269:PHE:CE2   | 2.36                     | 0.60              |
| 22:c:6028:CLA:H61  | 29:c:6057:DGD:HA42 | 1.84                     | 0.60              |
| 4:d:5221:THR:HG21  | 4:d:5245:SER:O     | 2.01                     | 0.60              |
| 10:k:5029:PRO:C    | 22:k:6034:CLA:O1D  | 2.45                     | 0.60              |
| 22:k:6034:CLA:O2A  | 22:k:6034:CLA:C1A  | 2.50                     | 0.60              |
| 13:o:5090:GLU:HA   | 13:o:5090:GLU:OE1  | 2.00                     | 0.60              |
| 15:u:5052:ASN:OD1  | 15:u:5064:ILE:HD13 | 2.02                     | 0.60              |
| 20:z:5032:ASP:HB3  | 20:z:5035:ARG:HG2  | 1.83                     | 0.60              |
| 1:A:244:GLU:HG2    | 4:D:264:LYS:NZ     | 2.17                     | 0.59              |
| 1:A:334:ARG:HB2    | 1:A:335:ASN:OD1    | 2.02                     | 0.59              |
| 22:A:1006:CLA:HAB  | 23:D:1039:PHO:C14  | 2.32                     | 0.59              |
| 2:B:188:ASP:OD1    | 2:B:191:ASN:HB2    | 2.02                     | 0.59              |
| 22:B:1009:CLA:CGA  | 22:B:1009:CLA:NA   | 2.64                     | 0.59              |
| 3:C:89:ILE:HA      | 3:C:92:ILE:HD13    | 1.83                     | 0.59              |
| 22:C:1026:CLA:C2B  | 22:C:1028:CLA:HBB2 | 2.32                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:C:1055:DGD:HB21 | 29:C:1055:DGD:C2A  | 2.30                     | 0.59              |
| 4:D:304:ARG:NH1    | 4:D:311:PHE:CD2    | 2.70                     | 0.59              |
| 7:H:30:LEU:O       | 7:H:33:VAL:HG22    | 2.02                     | 0.59              |
| 10:K:29:PRO:C      | 22:K:1034:CLA:O1D  | 2.45                     | 0.59              |
| 25:K:1051:BCR:C35  | 18:Y:32:GLY:HA3    | 2.21                     | 0.59              |
| 14:T:11:ALA:HB3    | 25:T:6046:BCR:H362 | 1.82                     | 0.59              |
| 1:a:5120:LEU:O     | 1:a:5120:LEU:HD13  | 2.02                     | 0.59              |
| 1:a:5279:ARG:CB    | 4:d:5212:ALA:HB2   | 2.31                     | 0.59              |
| 1:a:5330:VAL:HG11  | 4:d:5348:ARG:HG2   | 1.82                     | 0.59              |
| 22:b:6018:CLA:OBD  | 22:b:6018:CLA:C14  | 2.49                     | 0.59              |
| 3:c:5146:PHE:O     | 3:c:5148:GLY:N     | 2.34                     | 0.59              |
| 3:c:5160:ILE:HG21  | 22:c:6033:CLA:H202 | 1.85                     | 0.59              |
| 3:c:5353:GLY:HA3   | 3:c:5355:THR:HG23  | 1.84                     | 0.59              |
| 3:c:5458:GLY:HA3   | 4:d:5224:GLN:HB2   | 1.84                     | 0.59              |
| 22:c:6027:CLA:H3A  | 22:c:6027:CLA:O2A  | 2.02                     | 0.59              |
| 22:c:6035:CLA:H91  | 25:k:6052:BCR:H402 | 1.81                     | 0.59              |
| 4:d:5018:LEU:HD11  | 17:x:5037:LEU:HD13 | 1.83                     | 0.59              |
| 4:d:5199:MET:HA    | 4:d:5202:ALA:HB3   | 1.83                     | 0.59              |
| 15:u:5027:LEU:HD21 | 15:u:5082:PHE:HD1  | 1.65                     | 0.59              |
| 20:z:5027:TYR:N    | 20:z:5027:TYR:CD2  | 2.70                     | 0.59              |
| 20:z:5049:ALA:O    | 20:z:5053:VAL:HG23 | 2.01                     | 0.59              |
| 2:B:264:PRO:HG3    | 2:B:267:LEU:HB2    | 1.83                     | 0.59              |
| 2:B:392:PHE:HA     | 2:B:397:VAL:CG2    | 2.32                     | 0.59              |
| 22:B:1018:CLA:H8   | 22:B:1023:CLA:CBA  | 2.32                     | 0.59              |
| 3:C:72:LEU:HD13    | 3:C:112:PHE:HB2    | 1.84                     | 0.59              |
| 3:C:118:HIS:O      | 3:C:121:SER:HB3    | 2.02                     | 0.59              |
| 22:C:1030:CLA:HBB1 | 22:C:1030:CLA:CHC  | 2.14                     | 0.59              |
| 22:C:1035:CLA:C2B  | 25:C:1052:BCR:C27  | 2.77                     | 0.59              |
| 4:D:199:MET:HA     | 4:D:202:ALA:HB3    | 1.83                     | 0.59              |
| 9:J:10:LEU:HD22    | 9:J:11:TRP:H       | 1.67                     | 0.59              |
| 22:K:1034:CLA:C4   | 22:K:1034:CLA:CBA  | 2.81                     | 0.59              |
| 13:O:70:CYS:HB2    | 13:O:105:ASP:HB2   | 1.84                     | 0.59              |
| 13:O:83:LYS:HD2    | 13:O:85:LYS:HE3    | 1.83                     | 0.59              |
| 15:U:35:PHE:HD1    | 15:U:46:ALA:CB     | 2.15                     | 0.59              |
| 16:V:109:ASP:HB3   | 16:V:111:GLU:H     | 1.67                     | 0.59              |
| 1:a:5256:GLY:HA2   | 1:a:5264:SER:HB2   | 1.84                     | 0.59              |
| 2:b:5015:ASP:CG    | 2:b:5015:ASP:O     | 2.45                     | 0.59              |
| 2:b:5334:ASP:OD2   | 2:b:5334:ASP:N     | 2.32                     | 0.59              |
| 2:b:5465:GLY:N     | 22:b:6019:CLA:HAC1 | 2.17                     | 0.59              |
| 22:b:6009:CLA:CMB  | 25:h:6049:BCR:C27  | 2.69                     | 0.59              |
| 25:b:6045:BCR:H23C | 25:b:6045:BCR:C38  | 2.06                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6026:CLA:C2B  | 22:c:6028:CLA:HBB2 | 2.32                     | 0.59              |
| 24:d:6042:PQ9:H243 | 24:d:6042:PQ9:H292 | 1.84                     | 0.59              |
| 8:i:5021:PHE:CD1   | 8:i:5024:LEU:HD12  | 2.38                     | 0.59              |
| 25:k:6052:BCR:HC8  | 25:k:6052:BCR:C33  | 2.31                     | 0.59              |
| 16:v:5028:GLU:OE2  | 16:v:5028:GLU:HA   | 2.02                     | 0.59              |
| 1:A:320:ILE:HG21   | 4:D:180:ARG:HG3    | 1.84                     | 0.59              |
| 2:B:55:MET:HE3     | 2:B:80:ILE:CG2     | 2.32                     | 0.59              |
| 2:B:465:GLY:N      | 22:B:1019:CLA:HAC1 | 2.17                     | 0.59              |
| 22:B:1021:CLA:HBC3 | 25:B:1047:BCR:H343 | 1.83                     | 0.59              |
| 28:B:1060:MGE:H6D1 | 4:D:269:PHE:CE2    | 2.36                     | 0.59              |
| 3:C:403:SER:O      | 3:C:406:SER:N      | 2.34                     | 0.59              |
| 4:D:122:LEU:H      | 4:D:122:LEU:HD22   | 1.66                     | 0.59              |
| 4:D:156:VAL:O      | 4:D:156:VAL:HG12   | 2.02                     | 0.59              |
| 4:D:173:PHE:CD1    | 23:D:1039:PHO:H13  | 2.36                     | 0.59              |
| 23:a:6038:PHO:C9   | 22:d:6005:CLA:C18  | 2.80                     | 0.59              |
| 3:c:5155:ASN:O     | 3:c:5158:THR:HG22  | 2.02                     | 0.59              |
| 4:d:5039:PRO:HB2   | 22:d:6008:CLA:CBB  | 2.32                     | 0.59              |
| 4:d:5122:LEU:H     | 4:d:5122:LEU:HD22  | 1.66                     | 0.59              |
| 4:d:5156:VAL:O     | 4:d:5156:VAL:HG12  | 2.02                     | 0.59              |
| 16:v:5109:ASP:HB3  | 16:v:5111:GLU:H    | 1.67                     | 0.59              |
| 22:A:1006:CLA:H91  | 22:D:1004:CLA:H171 | 1.84                     | 0.59              |
| 2:B:222:PRO:HB2    | 2:B:225:LEU:HD12   | 1.84                     | 0.59              |
| 22:B:1009:CLA:C3D  | 22:B:1010:CLA:HBB2 | 2.26                     | 0.59              |
| 3:C:97:TRP:O       | 3:C:99:VAL:HG23    | 2.02                     | 0.59              |
| 3:C:140:LEU:HD21   | 3:C:146:PHE:CE1    | 2.29                     | 0.59              |
| 3:C:269:GLU:OE1    | 3:C:447:ARG:HD2    | 2.02                     | 0.59              |
| 22:C:1030:CLA:CED  | 22:C:1030:CLA:CHA  | 2.81                     | 0.59              |
| 4:D:39:PRO:HB2     | 22:D:1008:CLA:CBB  | 2.32                     | 0.59              |
| 25:D:1050:BCR:C21  | 28:D:1059:MGE:H3A1 | 2.32                     | 0.59              |
| 13:O:144:LEU:HD13  | 13:O:259:VAL:HG11  | 1.84                     | 0.59              |
| 16:V:62:ALA:O      | 16:V:63:CYS:CB     | 2.48                     | 0.59              |
| 20:Z:32:ASP:HB3    | 20:Z:35:ARG:HG2    | 1.84                     | 0.59              |
| 1:a:5225:ARG:HA    | 2:b:5481:GLY:HA3   | 1.83                     | 0.59              |
| 1:a:5258:LEU:O     | 1:a:5259:ILE:HD12  | 2.01                     | 0.59              |
| 2:b:5097:ALA:C     | 2:b:5099:ALA:H     | 2.10                     | 0.59              |
| 2:b:5113:TRP:O     | 2:b:5115:TRP:N     | 2.36                     | 0.59              |
| 2:b:5222:PRO:HB2   | 2:b:5225:LEU:HD12  | 1.84                     | 0.59              |
| 2:b:5247:PHE:C     | 2:b:5247:PHE:CD1   | 2.81                     | 0.59              |
| 22:b:6019:CLA:HMD3 | 28:b:6060:MGE:C1G  | 2.32                     | 0.59              |
| 3:c:5072:LEU:HD13  | 3:c:5112:PHE:HB2   | 1.84                     | 0.59              |
| 3:c:5097:TRP:O     | 3:c:5099:VAL:HG23  | 2.02                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6036:CLA:HED2 | 22:c:6037:CLA:HBB2 | 1.84                     | 0.59              |
| 4:d:5055:VAL:HG21  | 4:d:5110:LEU:CD2   | 2.33                     | 0.59              |
| 6:f:5041:GLN:NE2   | 9:j:5031:GLY:HA3   | 2.16                     | 0.59              |
| 7:h:5030:LEU:O     | 7:h:5033:VAL:HG22  | 2.02                     | 0.59              |
| 10:k:5035:LEU:CA   | 10:k:5038:VAL:HG23 | 2.29                     | 0.59              |
| 11:l:5029:LEU:HB2  | 14:t:5009:ILE:CG2  | 2.29                     | 0.59              |
| 14:t:5004:ILE:CD1  | 14:t:5005:THR:N    | 2.62                     | 0.59              |
| 16:v:5149:PRO:HB3  | 16:v:5156:TRP:HD1  | 1.67                     | 0.59              |
| 1:A:120:LEU:O      | 1:A:120:LEU:HD13   | 2.02                     | 0.59              |
| 1:A:196:PRO:HB2    | 29:C:1057:DGD:C8A  | 2.26                     | 0.59              |
| 1:A:331:MET:O      | 1:A:332:HIS:C      | 2.44                     | 0.59              |
| 1:A:338:ASN:O      | 1:A:339:PHE:CD1    | 2.56                     | 0.59              |
| 2:B:450:TRP:CH2    | 22:B:1015:CLA:H2   | 2.37                     | 0.59              |
| 22:B:1023:CLA:HBC2 | 22:B:1023:CLA:CMC  | 2.33                     | 0.59              |
| 22:B:1023:CLA:H112 | 22:B:1024:CLA:H8   | 1.84                     | 0.59              |
| 3:C:261:ARG:HA     | 3:C:266:TRP:HZ2    | 1.67                     | 0.59              |
| 22:C:1026:CLA:CGA  | 22:C:1026:CLA:H42  | 2.31                     | 0.59              |
| 22:C:1029:CLA:H51  | 22:C:1029:CLA:NB   | 2.15                     | 0.59              |
| 4:D:18:LEU:HD11    | 17:X:37:LEU:HD13   | 1.83                     | 0.59              |
| 4:D:55:VAL:HG21    | 4:D:110:LEU:CD2    | 2.33                     | 0.59              |
| 7:H:55:LEU:HB2     | 7:H:58:VAL:HB      | 1.84                     | 0.59              |
| 18:Y:22:LEU:O      | 18:Y:25:ILE:HG12   | 2.02                     | 0.59              |
| 1:a:5129:ARG:HG2   | 1:a:5129:ARG:O     | 2.01                     | 0.59              |
| 1:a:5147:TYR:C     | 1:a:5150:PRO:HD2   | 2.27                     | 0.59              |
| 1:a:5159:LEU:HD21  | 29:c:6055:DGD:C7A  | 2.26                     | 0.59              |
| 2:b:5018:ARG:HB3   | 2:b:5115:TRP:CZ3   | 2.37                     | 0.59              |
| 2:b:5091:TRP:CG    | 22:b:6014:CLA:HBA2 | 2.37                     | 0.59              |
| 3:c:5229:ASN:N     | 3:c:5229:ASN:ND2   | 2.44                     | 0.59              |
| 3:c:5271:TYR:HE1   | 22:c:6031:CLA:HAC1 | 1.64                     | 0.59              |
| 3:c:5348:GLU:OE1   | 3:c:5373:ASN:HB3   | 2.02                     | 0.59              |
| 22:c:6027:CLA:HMC1 | 22:c:6027:CLA:HBC3 | 1.84                     | 0.59              |
| 22:c:6029:CLA:C5   | 22:c:6029:CLA:C1C  | 2.79                     | 0.59              |
| 22:c:6033:CLA:HMA3 | 22:k:6034:CLA:C2C  | 2.30                     | 0.59              |
| 4:d:5072:ASN:H     | 4:d:5075:THR:HB    | 1.68                     | 0.59              |
| 4:d:5304:ARG:NH1   | 4:d:5311:PHE:CD2   | 2.70                     | 0.59              |
| 4:d:5352:LEU:H     | 4:d:5352:LEU:CD2   | 2.15                     | 0.59              |
| 22:h:6017:CLA:O1A  | 22:h:6017:CLA:H3A  | 2.02                     | 0.59              |
| 13:o:5070:CYS:HB2  | 13:o:5105:ASP:HB2  | 1.84                     | 0.59              |
| 13:o:5144:LEU:HD13 | 13:o:5259:VAL:HG11 | 1.84                     | 0.59              |
| 18:y:5022:LEU:O    | 18:y:5025:ILE:HG12 | 2.02                     | 0.59              |
| 1:A:225:ARG:HA     | 2:B:481:GLY:HA3    | 1.83                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:18:ARG:HB3     | 2:B:115:TRP:CZ3    | 2.37                     | 0.59              |
| 2:B:353:GLU:O      | 2:B:373:LYS:HE3    | 2.03                     | 0.59              |
| 3:C:176:VAL:HG21   | 3:C:238:ILE:HG12   | 1.85                     | 0.59              |
| 4:D:108:GLY:O      | 4:D:110:LEU:N      | 2.36                     | 0.59              |
| 4:D:299:ILE:HG22   | 4:D:300:SER:N      | 2.17                     | 0.59              |
| 22:K:1034:CLA:O2A  | 22:K:1034:CLA:C1A  | 2.50                     | 0.59              |
| 11:L:32:SER:HA     | 12:M:11:THR:OG1    | 2.03                     | 0.59              |
| 13:O:148:VAL:HG23  | 13:O:172:PHE:HE2   | 1.66                     | 0.59              |
| 25:T:6046:BCR:H323 | 25:T:6046:BCR:C4   | 2.33                     | 0.59              |
| 1:a:5275:LEU:HB2   | 4:d:5215:GLY:HA3   | 1.85                     | 0.59              |
| 2:b:5052:LEU:HD11  | 2:b:5339:ALA:HA    | 1.85                     | 0.59              |
| 2:b:5450:TRP:CH2   | 22:b:6015:CLA:H2   | 2.37                     | 0.59              |
| 22:b:6021:CLA:HBC3 | 25:b:6047:BCR:H343 | 1.83                     | 0.59              |
| 3:c:5118:HIS:O     | 3:c:5121:SER:HB3   | 2.02                     | 0.59              |
| 3:c:5266:TRP:HE3   | 3:c:5271:TYR:OH    | 1.85                     | 0.59              |
| 3:c:5318:LEU:HD23  | 3:c:5328:VAL:HG11  | 1.83                     | 0.59              |
| 4:d:5219:GLU:OE1   | 4:d:5219:GLU:HA    | 2.01                     | 0.59              |
| 4:d:5299:ILE:HG22  | 4:d:5300:SER:N     | 2.17                     | 0.59              |
| 7:h:5028:THR:HB    | 7:h:5029:PRO:HD3   | 1.85                     | 0.59              |
| 8:i:5013:THR:O     | 8:i:5014:PHE:C     | 2.43                     | 0.59              |
| 1:A:192:ILE:HG12   | 1:A:293:MET:HE1    | 1.84                     | 0.59              |
| 1:A:337:HIS:O      | 4:D:350:ASN:O      | 2.20                     | 0.59              |
| 2:B:247:PHE:C      | 2:B:247:PHE:CD1    | 2.81                     | 0.59              |
| 2:B:267:LEU:C      | 2:B:268:PHE:HD1    | 2.10                     | 0.59              |
| 2:B:320:ALA:HB1    | 4:D:292:ASN:HD22   | 1.67                     | 0.59              |
| 22:B:1009:CLA:HBA1 | 22:B:1009:CLA:O1D  | 1.99                     | 0.59              |
| 22:B:1009:CLA:CMB  | 25:H:1049:BCR:C27  | 2.69                     | 0.59              |
| 22:B:1022:CLA:C1   | 22:B:1022:CLA:CHA  | 2.80                     | 0.59              |
| 3:C:155:ASN:O      | 3:C:158:THR:HG22   | 2.02                     | 0.59              |
| 3:C:348:GLU:OE1    | 3:C:373:ASN:HB3    | 2.02                     | 0.59              |
| 3:C:353:GLY:HA3    | 3:C:355:THR:HG23   | 1.84                     | 0.59              |
| 4:D:29:PHE:CE2     | 4:D:31:GLY:N       | 2.71                     | 0.59              |
| 4:D:35:ILE:O       | 4:D:39:PRO:HG3     | 2.01                     | 0.59              |
| 6:F:41:GLN:HA      | 6:F:41:GLN:OE1     | 2.03                     | 0.59              |
| 13:O:227:VAL:HG11  | 13:O:230:VAL:HG22  | 1.85                     | 0.59              |
| 16:V:28:GLU:HA     | 16:V:28:GLU:OE2    | 2.02                     | 0.59              |
| 20:Z:27:TYR:N      | 20:Z:27:TYR:CD2    | 2.70                     | 0.59              |
| 22:a:6007:CLA:OBD  | 22:a:6007:CLA:CED  | 2.39                     | 0.59              |
| 2:b:5267:LEU:C     | 2:b:5268:PHE:HD1   | 2.10                     | 0.59              |
| 2:b:5406:LEU:O     | 2:b:5407:ASN:O     | 2.20                     | 0.59              |
| 25:c:6054:BCR:C8   | 25:c:6054:BCR:C31  | 2.80                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:j:5010:LEU:HD22  | 9:j:5011:TRP:H     | 1.67                     | 0.59              |
| 1:A:81:ALA:CB      | 1:A:175:GLY:HA3    | 2.33                     | 0.59              |
| 2:B:6:TYR:OH       | 28:L:1061:MGE:H2D  | 2.01                     | 0.59              |
| 2:B:18:ARG:NH2     | 2:B:115:TRP:NE1    | 2.51                     | 0.59              |
| 22:B:1018:CLA:HBC3 | 22:B:1018:CLA:HHD  | 1.85                     | 0.59              |
| 29:B:1058:DGD:O2D  | 4:D:87:HIS:HB2     | 2.02                     | 0.59              |
| 3:C:65:GLY:HA3     | 3:C:119:LEU:HB2    | 1.85                     | 0.59              |
| 22:C:1025:CLA:H171 | 22:C:1031:CLA:H102 | 1.83                     | 0.59              |
| 25:C:1052:BCR:HC8  | 25:C:1052:BCR:C33  | 2.31                     | 0.59              |
| 4:D:160:TYR:HB3    | 4:D:161:PRO:HD3    | 1.83                     | 0.59              |
| 8:I:31:ASN:HB2     | 8:I:32:PRO:CD      | 2.31                     | 0.59              |
| 16:V:58:LEU:O      | 16:V:61:TYR:N      | 2.36                     | 0.59              |
| 18:Y:43:ARG:CD     | 18:Y:44:GLY:N      | 2.63                     | 0.59              |
| 3:c:5176:VAL:HG21  | 3:c:5238:ILE:HG12  | 1.85                     | 0.59              |
| 3:c:5276:LEU:HD23  | 3:c:5276:LEU:O     | 2.01                     | 0.59              |
| 22:c:6025:CLA:C9   | 25:c:6054:BCR:H373 | 2.29                     | 0.59              |
| 22:c:6030:CLA:CED  | 22:c:6030:CLA:CHA  | 2.81                     | 0.59              |
| 4:d:5299:ILE:O     | 4:d:5300:SER:C     | 2.46                     | 0.59              |
| 22:A:1003:CLA:HAB  | 22:D:1004:CLA:NB   | 2.18                     | 0.59              |
| 24:A:1043:PQ9:H452 | 28:D:1059:MGE:C9A  | 2.33                     | 0.59              |
| 22:B:1011:CLA:C2   | 22:B:1013:CLA:H92  | 2.21                     | 0.59              |
| 22:B:1011:CLA:C4D  | 22:B:1013:CLA:C2   | 2.80                     | 0.59              |
| 3:C:43:ILE:HG23    | 3:C:43:ILE:O       | 2.03                     | 0.59              |
| 22:C:1028:CLA:H61  | 29:C:1057:DGD:HA42 | 1.84                     | 0.59              |
| 22:C:1035:CLA:H91  | 25:C:1052:BCR:H402 | 1.81                     | 0.59              |
| 6:F:15:ILE:HG13    | 6:F:16:PHE:CD1     | 2.30                     | 0.59              |
| 10:K:28:ILE:HG13   | 25:K:1051:BCR:C31  | 2.33                     | 0.59              |
| 13:O:72:GLN:HA     | 13:O:103:SER:OG    | 2.02                     | 0.59              |
| 14:T:4:ILE:CD1     | 14:T:5:THR:N       | 2.61                     | 0.59              |
| 20:Z:27:TYR:HD2    | 20:Z:27:TYR:H      | 1.49                     | 0.59              |
| 1:a:5196:PRO:CA    | 1:a:5199:GLN:HG3   | 2.31                     | 0.59              |
| 1:a:5201:GLY:O     | 1:a:5205:VAL:HG12  | 2.01                     | 0.59              |
| 22:a:6003:CLA:HAB  | 22:d:6004:CLA:NB   | 2.18                     | 0.59              |
| 4:d:5029:PHE:CE2   | 4:d:5031:GLY:N     | 2.71                     | 0.59              |
| 4:d:5253:TRP:CA    | 4:d:5256:ILE:HG22  | 2.15                     | 0.59              |
| 1:A:133:LEU:O      | 1:A:137:LEU:HB2    | 2.03                     | 0.59              |
| 1:A:243:GLU:HB3    | 4:D:240:ALA:HB1    | 1.85                     | 0.59              |
| 2:B:127:ARG:CD     | 2:B:128:THR:HG23   | 2.32                     | 0.59              |
| 22:B:1015:CLA:H91  | 22:B:1015:CLA:C12  | 2.33                     | 0.59              |
| 3:C:266:TRP:HE3    | 3:C:271:TYR:OH     | 1.85                     | 0.59              |
| 3:C:430:HIS:HD1    | 3:C:430:HIS:H      | 1.51                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1027:CLA:O2A  | 22:C:1027:CLA:H3A  | 2.03                     | 0.59              |
| 25:C:1052:BCR:H341 | 25:K:1051:BCR:HC21 | 1.84                     | 0.59              |
| 4:D:72:ASN:O       | 4:D:76:VAL:HG22    | 2.03                     | 0.59              |
| 4:D:198:MET:HA     | 22:D:1005:CLA:OBD  | 2.03                     | 0.59              |
| 7:H:63:LYS:O       | 7:H:64:ALA:HB2     | 2.03                     | 0.59              |
| 16:V:105:PRO:HG3   | 16:V:115:ALA:HA    | 1.83                     | 0.59              |
| 16:V:149:PRO:HB3   | 16:V:156:TRP:HD1   | 1.67                     | 0.59              |
| 3:c:5322:GLN:NE2   | 3:c:5381:LYS:HA    | 2.18                     | 0.59              |
| 22:c:6027:CLA:H121 | 22:c:6027:CLA:H18  | 1.84                     | 0.59              |
| 4:d:5145:ALA:HB2   | 4:d:5272:LEU:HD11  | 1.85                     | 0.59              |
| 10:k:5028:ILE:HG13 | 25:k:6051:BCR:C31  | 2.33                     | 0.59              |
| 11:l:5032:SER:HA   | 12:m:5011:THR:OG1  | 2.03                     | 0.59              |
| 18:y:5043:ARG:O    | 18:y:5044:GLY:O    | 2.20                     | 0.59              |
| 1:A:151:LEU:HD21   | 29:C:1055:DGD:HBS2 | 1.83                     | 0.58              |
| 1:A:190:HIS:HE1    | 1:A:296:ASN:HD22   | 1.50                     | 0.58              |
| 22:B:1021:CLA:HED3 | 22:B:1021:CLA:CGA  | 2.32                     | 0.58              |
| 3:C:131:TYR:O      | 3:C:133:ALA:N      | 2.36                     | 0.58              |
| 3:C:225:VAL:HG23   | 3:C:226:SER:N      | 2.19                     | 0.58              |
| 3:C:371:GLY:O      | 13:O:33:TYR:HB2    | 2.03                     | 0.58              |
| 3:C:458:GLY:HA3    | 4:D:224:GLN:HB2    | 1.84                     | 0.58              |
| 3:C:458:GLY:CA     | 4:D:224:GLN:HB2    | 2.33                     | 0.58              |
| 22:C:1025:CLA:C1   | 22:C:1025:CLA:C3A  | 2.81                     | 0.58              |
| 22:C:1029:CLA:H51  | 22:C:1029:CLA:CHC  | 2.18                     | 0.58              |
| 4:D:251:ARG:HH22   | 4:D:255:GLN:HE22   | 1.49                     | 0.58              |
| 22:D:1008:CLA:CBC  | 22:D:1008:CLA:CMC  | 2.81                     | 0.58              |
| 13:O:105:ASP:OD1   | 13:O:106:GLN:N     | 2.36                     | 0.58              |
| 13:O:196:SER:O     | 13:O:198:ILE:HG22  | 2.03                     | 0.58              |
| 1:a:5259:ILE:HG23  | 4:d:5128:ARG:NH1   | 2.18                     | 0.58              |
| 22:a:6006:CLA:HAB  | 23:d:6039:PHO:C14  | 2.32                     | 0.58              |
| 2:b:5113:TRP:C     | 2:b:5115:TRP:H     | 2.11                     | 0.58              |
| 3:c:5167:VAL:HG12  | 3:c:5168:LEU:N     | 2.17                     | 0.58              |
| 3:c:5269:GLU:OE1   | 3:c:5447:ARG:HD2   | 2.02                     | 0.58              |
| 3:c:5279:LEU:O     | 3:c:5280:SER:C     | 2.44                     | 0.58              |
| 13:o:5172:PHE:HB2  | 13:o:5221:GLY:CA   | 2.33                     | 0.58              |
| 13:o:5194:TYR:O    | 13:o:5195:ASP:HB3  | 2.03                     | 0.58              |
| 16:v:5058:LEU:O    | 16:v:5061:TYR:N    | 2.36                     | 0.58              |
| 20:z:5036:SER:HA   | 20:z:5039:LEU:HG   | 1.85                     | 0.58              |
| 1:A:137:LEU:CB     | 1:A:139:MET:HE3    | 2.33                     | 0.58              |
| 1:A:142:TRP:HB3    | 3:C:443:TRP:CZ3    | 2.38                     | 0.58              |
| 1:A:142:TRP:HZ2    | 4:D:219:GLU:HG3    | 1.67                     | 0.58              |
| 1:A:149:ALA:HB1    | 1:A:283:VAL:HG12   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:59:GLY:CA      | 2:B:329:PRO:HB3    | 2.29                     | 0.58              |
| 2:B:113:TRP:O      | 2:B:115:TRP:N      | 2.36                     | 0.58              |
| 22:H:1017:CLA:O1A  | 22:H:1017:CLA:H3A  | 2.02                     | 0.58              |
| 8:I:21:PHE:CD1     | 8:I:24:LEU:HD12    | 2.37                     | 0.58              |
| 14:T:18:PHE:HD1    | 25:T:6046:BCR:C33  | 2.16                     | 0.58              |
| 1:a:5149:ALA:HB1   | 1:a:5283:VAL:HG12  | 1.85                     | 0.58              |
| 1:a:5213:ALA:HB3   | 23:d:6039:PHO:HBC1 | 1.84                     | 0.58              |
| 23:a:6038:PHO:HED2 | 4:d:5213:ILE:HD13  | 1.86                     | 0.58              |
| 2:b:5092:SER:O     | 2:b:5093:PHE:C     | 2.46                     | 0.58              |
| 2:b:5264:PRO:HG3   | 2:b:5267:LEU:HB2   | 1.83                     | 0.58              |
| 2:b:5392:PHE:HA    | 2:b:5397:VAL:CG2   | 2.32                     | 0.58              |
| 22:b:6009:CLA:HHC  | 22:b:6009:CLA:CBB  | 2.20                     | 0.58              |
| 22:b:6015:CLA:H91  | 22:b:6015:CLA:C12  | 2.33                     | 0.58              |
| 29:b:6058:DGD:O2D  | 4:d:5087:HIS:HB2   | 2.02                     | 0.58              |
| 3:c:5033:PHE:CD1   | 3:c:5033:PHE:N     | 2.71                     | 0.58              |
| 3:c:5051:GLY:O     | 3:c:5055:ALA:N     | 2.24                     | 0.58              |
| 22:c:6030:CLA:HMB3 | 22:c:6031:CLA:C1C  | 2.34                     | 0.58              |
| 4:d:5108:GLY:O     | 4:d:5110:LEU:N     | 2.36                     | 0.58              |
| 4:d:5325:ILE:O     | 4:d:5329:MET:HG2   | 2.02                     | 0.58              |
| 10:k:5024:VAL:HG21 | 18:y:5025:ILE:CG2  | 2.26                     | 0.58              |
| 10:k:5024:VAL:O    | 10:k:5027:VAL:HG23 | 2.03                     | 0.58              |
| 13:o:5120:THR:HG23 | 13:o:5154:SER:OG   | 2.03                     | 0.58              |
| 16:v:5081:ARG:HG3  | 16:v:5157:GLY:CA   | 2.33                     | 0.58              |
| 1:A:107:TYR:C      | 1:A:109:GLY:H      | 2.12                     | 0.58              |
| 2:B:3:LEU:HD22     | 11:L:8:GLN:HB2     | 1.84                     | 0.58              |
| 22:B:1016:CLA:C2   | 22:H:1017:CLA:H91  | 2.31                     | 0.58              |
| 22:B:1018:CLA:H102 | 22:B:1023:CLA:HBA2 | 1.85                     | 0.58              |
| 22:B:1023:CLA:C3C  | 22:B:1024:CLA:HBC1 | 2.33                     | 0.58              |
| 3:C:171:GLY:O      | 3:C:174:LEU:N      | 2.36                     | 0.58              |
| 3:C:443:TRP:HD1    | 22:C:1032:CLA:HMD3 | 1.68                     | 0.58              |
| 13:O:77:LEU:CD2    | 13:O:93:PRO:HA     | 2.33                     | 0.58              |
| 13:O:144:LEU:CD1   | 13:O:259:VAL:HG11  | 2.34                     | 0.58              |
| 18:Y:43:ARG:O      | 18:Y:44:GLY:O      | 2.21                     | 0.58              |
| 1:a:5121:LEU:O     | 1:a:5123:ALA:N     | 2.36                     | 0.58              |
| 1:a:5183:MET:HB3   | 22:a:6003:CLA:CBC  | 2.27                     | 0.58              |
| 1:a:5192:ILE:HG12  | 1:a:5293:MET:HE1   | 1.84                     | 0.58              |
| 2:b:5003:LEU:HD22  | 11:l:5008:GLN:HB2  | 1.84                     | 0.58              |
| 2:b:5018:ARG:NH2   | 2:b:5115:TRP:NE1   | 2.51                     | 0.58              |
| 2:b:5092:SER:O     | 2:b:5095:GLY:N     | 2.37                     | 0.58              |
| 2:b:5246:PHE:C     | 2:b:5246:PHE:CD1   | 2.81                     | 0.58              |
| 2:b:5320:ALA:HB1   | 4:d:5292:ASN:HD22  | 1.67                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5261:ARG:HA    | 3:c:5266:TRP:HZ2   | 1.67                     | 0.58              |
| 3:c:5458:GLY:CA    | 4:d:5224:GLN:HB2   | 2.33                     | 0.58              |
| 22:c:6025:CLA:H143 | 25:c:6054:BCR:C35  | 2.33                     | 0.58              |
| 13:o:5155:THR:HG22 | 13:o:5167:ASP:O    | 2.03                     | 0.58              |
| 13:o:5223:ILE:HD13 | 13:o:5225:LEU:HD13 | 1.83                     | 0.58              |
| 1:A:30:VAL:O       | 1:A:30:VAL:HG22    | 2.02                     | 0.58              |
| 1:A:275:LEU:HB2    | 4:D:215:GLY:HA3    | 1.85                     | 0.58              |
| 2:B:92:SER:O       | 2:B:95:GLY:N       | 2.36                     | 0.58              |
| 3:C:87:ILE:HG22    | 3:C:426:LEU:HD11   | 1.83                     | 0.58              |
| 3:C:322:GLN:NE2    | 3:C:381:LYS:HA     | 2.18                     | 0.58              |
| 29:C:1057:DGD:HGB3 | 29:C:1057:DGD:CEB  | 2.21                     | 0.58              |
| 4:D:87:HIS:HA      | 4:D:167:TRP:CD1    | 2.38                     | 0.58              |
| 4:D:152:VAL:HG21   | 4:D:279:LEU:HD22   | 1.86                     | 0.58              |
| 1:a:5137:LEU:CB    | 1:a:5139:MET:HE3   | 2.33                     | 0.58              |
| 1:a:5256:GLY:O     | 1:a:5261:GLN:N     | 2.36                     | 0.58              |
| 22:a:6003:CLA:CED  | 22:a:6003:CLA:C2A  | 2.64                     | 0.58              |
| 2:b:5055:MET:CE    | 2:b:5080:ILE:HG21  | 2.33                     | 0.58              |
| 22:c:6029:CLA:HHC  | 22:c:6029:CLA:CBB  | 2.32                     | 0.58              |
| 22:c:6031:CLA:OBD  | 22:c:6033:CLA:C16  | 2.48                     | 0.58              |
| 4:d:5148:ALA:HB2   | 4:d:5276:VAL:HG12  | 1.84                     | 0.58              |
| 6:f:5015:ILE:HG13  | 6:f:5016:PHE:CD1   | 2.30                     | 0.58              |
| 6:f:5041:GLN:OE1   | 6:f:5041:GLN:HA    | 2.03                     | 0.58              |
| 25:k:6052:BCR:H341 | 25:k:6051:BCR:HC21 | 1.84                     | 0.58              |
| 1:A:183:MET:HB3    | 22:A:1003:CLA:CBC  | 2.27                     | 0.58              |
| 2:B:191:ASN:HD22   | 7:H:60:VAL:HG12    | 1.67                     | 0.58              |
| 2:B:311:PHE:CE2    | 2:B:317:ASN:ND2    | 2.64                     | 0.58              |
| 2:B:442:ILE:HD11   | 13:O:200:LEU:CD2   | 2.33                     | 0.58              |
| 3:C:128:GLY:HA3    | 22:C:1037:CLA:CAC  | 2.33                     | 0.58              |
| 3:C:289:PHE:O      | 3:C:289:PHE:HD2    | 1.87                     | 0.58              |
| 22:C:1030:CLA:HMB3 | 22:C:1031:CLA:C1C  | 2.34                     | 0.58              |
| 22:C:1036:CLA:HED2 | 22:C:1037:CLA:HBB2 | 1.84                     | 0.58              |
| 4:D:33:SER:O       | 4:D:35:ILE:N       | 2.36                     | 0.58              |
| 4:D:53:THR:HA      | 4:D:67:TYR:HD2     | 1.69                     | 0.58              |
| 4:D:110:LEU:O      | 4:D:113:PHE:HB3    | 2.04                     | 0.58              |
| 10:K:24:VAL:O      | 10:K:27:VAL:HG23   | 2.03                     | 0.58              |
| 13:O:79:LYS:HE2    | 13:O:89:ALA:CB     | 2.33                     | 0.58              |
| 13:O:172:PHE:HB2   | 13:O:221:GLY:CA    | 2.33                     | 0.58              |
| 18:Y:39:LEU:HD21   | 20:Z:28:ALA:HB3    | 1.86                     | 0.58              |
| 1:a:5133:LEU:O     | 1:a:5137:LEU:HB2   | 2.03                     | 0.58              |
| 1:a:5202:VAL:HG11  | 22:a:6006:CLA:CAD  | 2.33                     | 0.58              |
| 2:b:5284:ILE:CG2   | 2:b:5305:ILE:HD13  | 2.34                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6023:CLA:H112 | 22:b:6024:CLA:H8   | 1.84                     | 0.58              |
| 3:c:5171:GLY:C     | 3:c:5173:LEU:N     | 2.59                     | 0.58              |
| 4:d:5198:MET:HA    | 22:d:6005:CLA:OBD  | 2.03                     | 0.58              |
| 22:d:6008:CLA:CBC  | 22:d:6008:CLA:CMC  | 2.82                     | 0.58              |
| 8:i:5024:LEU:O     | 8:i:5026:GLY:N     | 2.37                     | 0.58              |
| 15:u:5058:VAL:O    | 15:u:5061:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:213:ALA:HB2    | 4:D:275:PRO:HG2    | 1.85                     | 0.58              |
| 3:C:121:SER:O      | 3:C:125:LEU:HD12   | 2.04                     | 0.58              |
| 22:D:1004:CLA:C14  | 22:D:1004:CLA:H102 | 2.34                     | 0.58              |
| 5:E:22:ILE:HG23    | 19:N:18:UNK:HA     | 1.86                     | 0.58              |
| 5:E:57:ALA:HB3     | 5:E:60:GLN:CG      | 2.33                     | 0.58              |
| 7:H:28:THR:HB      | 7:H:29:PRO:HD3     | 1.85                     | 0.58              |
| 1:a:5030:VAL:O     | 1:a:5030:VAL:HG22  | 2.02                     | 0.58              |
| 1:a:5142:TRP:HB3   | 3:c:5443:TRP:CZ3   | 2.37                     | 0.58              |
| 22:b:6018:CLA:H8   | 22:b:6023:CLA:CBA  | 2.32                     | 0.58              |
| 22:b:6018:CLA:HBC3 | 22:b:6018:CLA:HHD  | 1.85                     | 0.58              |
| 3:c:5348:GLU:CD    | 3:c:5349:ILE:HG13  | 2.28                     | 0.58              |
| 22:c:6028:CLA:C2   | 29:c:6056:DGD:O1A  | 2.46                     | 0.58              |
| 9:j:5010:LEU:HD13  | 9:j:5010:LEU:N     | 2.14                     | 0.58              |
| 22:k:6034:CLA:C4   | 22:k:6034:CLA:CBA  | 2.81                     | 0.58              |
| 13:o:5107:ILE:HG23 | 13:o:5123:GLU:HG3  | 1.84                     | 0.58              |
| 13:o:5144:LEU:CD1  | 13:o:5259:VAL:HG11 | 2.34                     | 0.58              |
| 15:u:5061:VAL:CG1  | 15:u:5075:LEU:HD23 | 2.32                     | 0.58              |
| 1:A:121:LEU:O      | 1:A:123:ALA:N      | 2.36                     | 0.58              |
| 3:C:42:LEU:HD12    | 3:C:48:LYS:HG2     | 1.85                     | 0.58              |
| 3:C:143:TYR:CD1    | 3:C:143:TYR:O      | 2.57                     | 0.58              |
| 22:C:1025:CLA:C4   | 22:C:1025:CLA:C1B  | 2.77                     | 0.58              |
| 22:C:1025:CLA:H143 | 25:C:1054:BCR:C35  | 2.33                     | 0.58              |
| 25:C:1054:BCR:C8   | 25:C:1054:BCR:C31  | 2.80                     | 0.58              |
| 4:D:189:HIS:HA     | 4:D:294:ARG:HD2    | 1.85                     | 0.58              |
| 4:D:330:ALA:N      | 4:D:331:PRO:HD2    | 2.19                     | 0.58              |
| 13:O:155:THR:HG22  | 13:O:167:ASP:O     | 2.03                     | 0.58              |
| 25:T:6048:BCR:C8   | 25:T:6048:BCR:C33  | 2.81                     | 0.58              |
| 16:V:62:ALA:O      | 31:V:1041:HEM:HBB1 | 2.04                     | 0.58              |
| 1:a:5081:ALA:CB    | 1:a:5175:GLY:HA3   | 2.33                     | 0.58              |
| 1:a:5114:LEU:HD22  | 22:a:6007:CLA:HED3 | 1.86                     | 0.58              |
| 1:a:5200:LEU:HD23  | 29:c:6057:DGD:HBW2 | 1.86                     | 0.58              |
| 1:a:5309:ALA:CB    | 16:v:5028:GLU:HB2  | 2.34                     | 0.58              |
| 26:a:6063:LHG:H292 | 22:c:6032:CLA:C5   | 2.26                     | 0.58              |
| 2:b:5353:GLU:O     | 2:b:5373:LYS:HE3   | 2.03                     | 0.58              |
| 22:b:6022:CLA:C1   | 22:b:6022:CLA:CHA  | 2.80                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5043:ILE:HG23  | 3:c:5043:ILE:O     | 2.03                     | 0.58              |
| 3:c:5171:GLY:O     | 3:c:5174:LEU:N     | 2.36                     | 0.58              |
| 22:c:6025:CLA:H3A  | 22:c:6025:CLA:CGA  | 2.28                     | 0.58              |
| 4:d:5018:LEU:HD23  | 4:d:5032:TRP:HH2   | 1.68                     | 0.58              |
| 4:d:5072:ASN:O     | 4:d:5076:VAL:HG22  | 2.03                     | 0.58              |
| 7:h:5063:LYS:O     | 7:h:5064:ALA:HB2   | 2.03                     | 0.58              |
| 15:u:5035:PHE:HD1  | 15:u:5046:ALA:CB   | 2.15                     | 0.58              |
| 16:v:5038:LEU:HB2  | 16:v:5045:ILE:CG1  | 2.34                     | 0.58              |
| 22:B:1022:CLA:O2A  | 22:B:1022:CLA:CHA  | 2.52                     | 0.58              |
| 3:C:33:PHE:N       | 3:C:33:PHE:CD1     | 2.71                     | 0.58              |
| 22:D:1004:CLA:H201 | 28:D:1059:MGE:C8A  | 2.32                     | 0.58              |
| 5:E:28:PRO:O       | 5:E:32:ILE:HB      | 2.04                     | 0.58              |
| 15:U:59:GLU:C      | 15:U:61:VAL:N      | 2.58                     | 0.58              |
| 20:Z:36:SER:HA     | 20:Z:39:LEU:HG     | 1.85                     | 0.58              |
| 1:a:5243:GLU:HB3   | 4:d:5240:ALA:HB1   | 1.85                     | 0.58              |
| 3:c:5033:PHE:CE2   | 3:c:5040:ALA:HB1   | 2.39                     | 0.58              |
| 22:c:6025:CLA:C1   | 22:c:6025:CLA:C3A  | 2.81                     | 0.58              |
| 22:c:6029:CLA:C1C  | 22:c:6029:CLA:C3   | 2.82                     | 0.58              |
| 4:d:5033:SER:O     | 4:d:5035:ILE:N     | 2.36                     | 0.58              |
| 5:e:5028:PRO:O     | 5:e:5032:ILE:HB    | 2.04                     | 0.58              |
| 13:o:5077:LEU:CD2  | 13:o:5093:PRO:HA   | 2.33                     | 0.58              |
| 16:v:5062:ALA:O    | 31:v:6041:HEM:HBB1 | 2.04                     | 0.58              |
| 16:v:5109:ASP:HB3  | 16:v:5111:GLU:HB2  | 1.85                     | 0.58              |
| 1:A:309:ALA:CB     | 16:V:28:GLU:HB2    | 2.34                     | 0.58              |
| 23:A:1038:PHO:CHD  | 23:A:1038:PHO:CBC  | 2.81                     | 0.58              |
| 2:B:92:SER:O       | 2:B:93:PHE:C       | 2.46                     | 0.58              |
| 2:B:153:PHE:CD1    | 2:B:157:HIS:HB3    | 2.39                     | 0.58              |
| 2:B:193:TYR:O      | 2:B:261:ALA:HB2    | 2.03                     | 0.58              |
| 3:C:33:PHE:CE2     | 3:C:40:ALA:HB1     | 2.39                     | 0.58              |
| 3:C:239:TRP:O      | 3:C:243:ILE:HG13   | 2.04                     | 0.58              |
| 22:C:1036:CLA:HHC  | 22:C:1036:CLA:CBB  | 2.29                     | 0.58              |
| 4:D:18:LEU:HD23    | 4:D:32:TRP:HH2     | 1.68                     | 0.58              |
| 4:D:72:ASN:H       | 4:D:75:THR:HB      | 1.68                     | 0.58              |
| 4:D:299:ILE:O      | 4:D:300:SER:C      | 2.46                     | 0.58              |
| 6:F:20:TRP:NE1     | 6:F:24:HIS:CE1     | 2.72                     | 0.58              |
| 12:M:32:GLN:CD     | 12:m:5034:LYS:HD2  | 2.29                     | 0.58              |
| 13:O:120:THR:HG23  | 13:O:154:SER:OG    | 2.03                     | 0.58              |
| 15:U:68:THR:HG22   | 15:U:71:GLN:HB2    | 1.85                     | 0.58              |
| 1:a:5032:TRP:O     | 1:a:5035:VAL:HG12  | 2.04                     | 0.58              |
| 2:b:5179:GLN:HB3   | 2:b:5180:PRO:HD2   | 1.86                     | 0.58              |
| 2:b:5331:ASN:C     | 2:b:5333:GLY:H     | 2.12                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5442:ILE:HD11  | 13:o:5200:LEU:CD2  | 2.33                     | 0.58              |
| 3:c:5225:VAL:HG23  | 3:c:5226:SER:N     | 2.19                     | 0.58              |
| 4:d:5330:ALA:N     | 4:d:5331:PRO:HD2   | 2.19                     | 0.58              |
| 5:e:5057:ALA:HB3   | 5:e:5060:GLN:CG    | 2.33                     | 0.58              |
| 11:l:5031:PHE:O    | 11:l:5032:SER:C    | 2.47                     | 0.58              |
| 13:o:5188:ARG:HB2  | 13:o:5188:ARG:HH11 | 1.68                     | 0.58              |
| 18:y:5044:GLY:O    | 18:y:5045:ASN:CB   | 2.49                     | 0.58              |
| 1:A:202:VAL:HG11   | 22:A:1006:CLA:CAD  | 2.33                     | 0.58              |
| 1:A:325:ASN:HD22   | 1:A:328:MET:CE     | 2.14                     | 0.58              |
| 23:A:1038:PHO:HED2 | 4:D:213:ILE:HD13   | 1.86                     | 0.58              |
| 2:B:55:MET:CE      | 2:B:80:ILE:HG21    | 2.33                     | 0.58              |
| 2:B:113:TRP:C      | 2:B:115:TRP:H      | 2.11                     | 0.58              |
| 2:B:246:PHE:CD1    | 2:B:246:PHE:C      | 2.81                     | 0.58              |
| 3:C:143:TYR:O      | 3:C:143:TYR:HD1    | 1.86                     | 0.58              |
| 3:C:223:TRP:CD1    | 3:C:224:ILE:CD1    | 2.87                     | 0.58              |
| 3:C:287:THR:OG1    | 3:C:430:HIS:HB2    | 2.04                     | 0.58              |
| 22:C:1027:CLA:H121 | 22:C:1027:CLA:H18  | 1.84                     | 0.58              |
| 4:D:145:ALA:HB2    | 4:D:272:LEU:HD11   | 1.85                     | 0.58              |
| 4:D:222:LEU:HD21   | 4:D:243:THR:OG1    | 2.04                     | 0.58              |
| 10:K:28:ILE:O      | 10:K:31:LEU:HB2    | 2.04                     | 0.58              |
| 10:K:28:ILE:HA     | 10:K:31:LEU:HD12   | 1.86                     | 0.58              |
| 13:O:172:PHE:HB2   | 13:O:221:GLY:HA3   | 1.85                     | 0.58              |
| 13:O:194:TYR:O     | 13:O:195:ASP:HB3   | 2.03                     | 0.58              |
| 15:U:52:ASN:O      | 15:U:53:ALA:O      | 2.22                     | 0.58              |
| 15:U:75:LEU:HD12   | 15:U:75:LEU:H      | 1.69                     | 0.58              |
| 16:V:81:ARG:HG3    | 16:V:157:GLY:CA    | 2.33                     | 0.58              |
| 1:a:5078:ILE:HA    | 1:a:5176:ILE:HD12  | 1.86                     | 0.58              |
| 22:b:6018:CLA:H102 | 22:b:6023:CLA:HBA2 | 1.85                     | 0.58              |
| 3:c:5042:LEU:HG    | 22:c:6035:CLA:HMA1 | 1.86                     | 0.58              |
| 3:c:5143:TYR:O     | 3:c:5143:TYR:HD1   | 1.86                     | 0.58              |
| 3:c:5289:PHE:HD2   | 3:c:5289:PHE:O     | 1.87                     | 0.58              |
| 3:c:5330:SER:C     | 13:o:5129:PHE:HE1  | 2.11                     | 0.58              |
| 4:d:5189:HIS:HA    | 4:d:5294:ARG:HD2   | 1.85                     | 0.58              |
| 22:d:6004:CLA:HBD  | 22:d:6004:CLA:HAA2 | 1.86                     | 0.58              |
| 13:o:5105:ASP:OD1  | 13:o:5106:GLN:N    | 2.36                     | 0.58              |
| 13:o:5172:PHE:HB2  | 13:o:5221:GLY:HA3  | 1.85                     | 0.58              |
| 15:u:5075:LEU:HD12 | 15:u:5075:LEU:H    | 1.69                     | 0.58              |
| 1:A:94:TYR:OH      | 1:A:104:GLU:HG2    | 2.04                     | 0.57              |
| 1:A:197:PHE:CE1    | 1:A:285:PHE:HD2    | 2.18                     | 0.57              |
| 2:B:74:SER:C       | 2:B:76:SER:H       | 2.12                     | 0.57              |
| 2:B:179:GLN:HB3    | 2:B:180:PRO:HD2    | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:284:ILE:CG2    | 2:B:305:ILE:HD13   | 2.34                     | 0.57              |
| 22:B:1012:CLA:CMD  | 22:B:1020:CLA:C20  | 2.78                     | 0.57              |
| 22:C:1027:CLA:HMC1 | 22:C:1027:CLA:HBC3 | 1.84                     | 0.57              |
| 22:C:1028:CLA:C2   | 29:C:1056:DGD:O1A  | 2.46                     | 0.57              |
| 22:C:1033:CLA:CMA  | 22:K:1034:CLA:CMC  | 2.80                     | 0.57              |
| 22:D:1004:CLA:HAA2 | 22:D:1004:CLA:HBD  | 1.86                     | 0.57              |
| 9:J:7:ARG:HG2      | 9:J:7:ARG:HH11     | 1.69                     | 0.57              |
| 14:T:1:MET:HE2     | 14:T:2:GLU:HG3     | 1.85                     | 0.57              |
| 1:a:5172:MET:HE2   | 1:a:5179:THR:HB    | 1.85                     | 0.57              |
| 1:a:5213:ALA:HB2   | 4:d:5275:PRO:HG2   | 1.85                     | 0.57              |
| 2:b:5003:LEU:HD22  | 11:l:5008:GLN:CB   | 2.34                     | 0.57              |
| 2:b:5083:GLU:CG    | 2:b:5086:ILE:HD11  | 2.31                     | 0.57              |
| 2:b:5096:VAL:O     | 2:b:5099:ALA:HB3   | 2.04                     | 0.57              |
| 2:b:5153:PHE:CD1   | 2:b:5157:HIS:HB3   | 2.39                     | 0.57              |
| 2:b:5191:ASN:HD22  | 7:h:5060:VAL:HG12  | 1.67                     | 0.57              |
| 2:b:5229:LEU:O     | 2:b:5231:MET:N     | 2.37                     | 0.57              |
| 3:c:5128:GLY:HA3   | 22:c:6037:CLA:CAC  | 2.33                     | 0.57              |
| 3:c:5143:TYR:O     | 3:c:5143:TYR:CD1   | 2.57                     | 0.57              |
| 22:c:6030:CLA:H171 | 22:c:6030:CLA:C14  | 2.21                     | 0.57              |
| 22:c:6036:CLA:HBC2 | 22:c:6036:CLA:CMC  | 2.34                     | 0.57              |
| 4:d:5152:VAL:HG21  | 4:d:5279:LEU:HD22  | 1.86                     | 0.57              |
| 4:d:5214:HIS:HA    | 4:d:5217:THR:HG22  | 1.86                     | 0.57              |
| 9:j:5015:THR:HG21  | 10:k:5038:VAL:CG1  | 2.34                     | 0.57              |
| 12:m:5019:SER:O    | 12:m:5023:ILE:HG12 | 2.04                     | 0.57              |
| 13:o:5196:SER:O    | 13:o:5198:ILE:HG22 | 2.03                     | 0.57              |
| 15:u:5068:THR:HG22 | 15:u:5071:GLN:HB2  | 1.85                     | 0.57              |
| 1:A:45:THR:HG23    | 1:A:46:ILE:H       | 1.68                     | 0.57              |
| 1:A:78:ILE:HA      | 1:A:176:ILE:HD12   | 1.86                     | 0.57              |
| 1:A:259:ILE:HG23   | 4:D:128:ARG:NH1    | 2.18                     | 0.57              |
| 2:B:97:ALA:C       | 2:B:99:ALA:H       | 2.10                     | 0.57              |
| 22:B:1016:CLA:H193 | 22:H:1017:CLA:C19  | 2.15                     | 0.57              |
| 3:C:167:VAL:HG12   | 3:C:168:LEU:N      | 2.17                     | 0.57              |
| 3:C:369:LEU:HD11   | 3:C:384:ILE:HG13   | 1.86                     | 0.57              |
| 22:C:1029:CLA:C1C  | 22:C:1029:CLA:C3   | 2.82                     | 0.57              |
| 15:U:58:VAL:O      | 15:U:61:VAL:HG23   | 2.03                     | 0.57              |
| 17:X:43:ILE:O      | 17:X:43:ILE:CG2    | 2.52                     | 0.57              |
| 1:a:5094:TYR:OH    | 1:a:5104:GLU:HG2   | 2.04                     | 0.57              |
| 2:b:5251:VAL:HG13  | 22:b:6010:CLA:H2   | 1.86                     | 0.57              |
| 22:b:6009:CLA:O1A  | 22:b:6009:CLA:C4D  | 2.53                     | 0.57              |
| 22:b:6023:CLA:HBC2 | 22:b:6023:CLA:CMC  | 2.33                     | 0.57              |
| 3:c:5065:GLY:HA3   | 3:c:5119:LEU:HB2   | 1.85                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5369:LEU:HD11  | 3:c:5384:ILE:HG13  | 1.86                     | 0.57              |
| 4:d:5110:LEU:O     | 4:d:5113:PHE:HB3   | 2.04                     | 0.57              |
| 13:o:5227:VAL:HG11 | 13:o:5230:VAL:HG22 | 1.85                     | 0.57              |
| 16:v:5038:LEU:CB   | 16:v:5045:ILE:HD11 | 2.33                     | 0.57              |
| 1:A:256:GLY:O      | 1:A:261:GLN:N      | 2.36                     | 0.57              |
| 1:A:279:ARG:HG2    | 4:D:212:ALA:HB2    | 1.86                     | 0.57              |
| 2:B:226:TYR:HA     | 2:B:231:MET:SD     | 2.45                     | 0.57              |
| 2:B:229:LEU:O      | 2:B:231:MET:N      | 2.37                     | 0.57              |
| 22:B:1009:CLA:O1A  | 22:B:1009:CLA:C4D  | 2.53                     | 0.57              |
| 22:C:1031:CLA:CAD  | 22:C:1033:CLA:H161 | 2.34                     | 0.57              |
| 4:D:266:TRP:CD1    | 28:D:1062:MGE:H2D  | 2.39                     | 0.57              |
| 12:M:19:SER:O      | 12:M:23:ILE:HG12   | 2.04                     | 0.57              |
| 12:M:34:LYS:HA     | 12:m:5032:GLN:HE22 | 1.69                     | 0.57              |
| 15:U:61:VAL:CG1    | 15:U:75:LEU:HD23   | 2.32                     | 0.57              |
| 15:U:69:GLU:HA     | 15:U:72:LYS:HE3    | 1.86                     | 0.57              |
| 16:V:38:LEU:CA     | 16:V:95:ILE:HG22   | 2.28                     | 0.57              |
| 25:Z:1053:BCR:C38  | 25:Z:1053:BCR:C23  | 2.59                     | 0.57              |
| 1:a:5104:GLU:OE1   | 13:o:5099:ARG:HD2  | 2.04                     | 0.57              |
| 24:a:6043:PQ9:H452 | 28:d:6059:MGE:C9A  | 2.33                     | 0.57              |
| 2:b:5020:ILE:O     | 2:b:5024:LEU:HB2   | 2.04                     | 0.57              |
| 2:b:5122:LEU:HD23  | 7:h:5008:GLY:HA2   | 1.87                     | 0.57              |
| 22:b:6012:CLA:CMD  | 22:b:6020:CLA:C20  | 2.78                     | 0.57              |
| 22:b:6016:CLA:H162 | 22:d:6008:CLA:HMA3 | 1.70                     | 0.57              |
| 22:b:6016:CLA:HAB  | 4:d:5123:ILE:HG23  | 1.86                     | 0.57              |
| 3:c:5131:TYR:O     | 3:c:5133:ALA:N     | 2.36                     | 0.57              |
| 3:c:5223:TRP:CD1   | 3:c:5224:ILE:CD1   | 2.87                     | 0.57              |
| 3:c:5287:THR:OG1   | 3:c:5430:HIS:HB2   | 2.04                     | 0.57              |
| 3:c:5465:PRO:HG2   | 8:i:5032:PRO:HB3   | 1.87                     | 0.57              |
| 22:c:6032:CLA:H2   | 22:k:6034:CLA:HMB1 | 1.87                     | 0.57              |
| 4:d:5103:ARG:HD2   | 5:e:5076:VAL:HG21  | 1.84                     | 0.57              |
| 4:d:5110:LEU:HD12  | 4:d:5110:LEU:H     | 1.70                     | 0.57              |
| 6:f:5020:TRP:NE1   | 6:f:5024:HIS:CE1   | 2.72                     | 0.57              |
| 14:t:5001:MET:HE2  | 14:t:5002:GLU:HG3  | 1.85                     | 0.57              |
| 18:y:5043:ARG:HD2  | 18:y:5044:GLY:N    | 2.19                     | 0.57              |
| 1:A:32:TRP:O       | 1:A:35:VAL:HG12    | 2.04                     | 0.57              |
| 1:A:114:LEU:HD22   | 22:A:1007:CLA:HED3 | 1.86                     | 0.57              |
| 1:A:172:MET:HE2    | 1:A:179:THR:HB     | 1.85                     | 0.57              |
| 1:A:192:ILE:CD1    | 1:A:198:HIS:HB2    | 2.34                     | 0.57              |
| 2:B:52:LEU:HD11    | 2:B:339:ALA:HA     | 1.85                     | 0.57              |
| 2:B:331:ASN:C      | 2:B:333:GLY:H      | 2.12                     | 0.57              |
| 22:B:1010:CLA:HBD  | 22:B:1010:CLA:H11  | 1.81                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1012:CLA:HAA1 | 22:B:1012:CLA:HBD  | 1.86                     | 0.57              |
| 3:C:330:SER:C      | 13:O:129:PHE:HE1   | 2.11                     | 0.57              |
| 4:D:89:LEU:HB2     | 4:D:91:LEU:CD1     | 2.35                     | 0.57              |
| 4:D:193:LEU:O      | 4:D:193:LEU:HD23   | 2.04                     | 0.57              |
| 4:D:297:ASP:CG     | 4:D:298:PHE:N      | 2.59                     | 0.57              |
| 31:F:1040:HEM:HMB2 | 31:F:1040:HEM:CBB  | 2.32                     | 0.57              |
| 16:V:109:ASP:HB3   | 16:V:111:GLU:HB2   | 1.85                     | 0.57              |
| 1:a:5167:SER:C     | 1:a:5169:SER:N     | 2.61                     | 0.57              |
| 1:a:5336:ALA:O     | 1:a:5338:ASN:N     | 2.36                     | 0.57              |
| 22:b:6010:CLA:HED3 | 22:b:6011:CLA:HMA2 | 1.86                     | 0.57              |
| 22:b:6019:CLA:HHC  | 22:b:6019:CLA:CBB  | 2.34                     | 0.57              |
| 3:c:5350:ILE:HG21  | 3:c:5359:TRP:CB    | 2.28                     | 0.57              |
| 4:d:5087:HIS:HA    | 4:d:5167:TRP:CD1   | 2.38                     | 0.57              |
| 10:k:5033:PHE:HE1  | 10:k:5037:PHE:CE2  | 2.22                     | 0.57              |
| 15:u:5052:ASN:O    | 15:u:5053:ALA:O    | 2.22                     | 0.57              |
| 1:A:184:ILE:CG1    | 4:D:186:GLN:NE2    | 2.66                     | 0.57              |
| 2:B:9:HIS:CG       | 22:B:1020:CLA:HBB2 | 2.40                     | 0.57              |
| 2:B:20:ILE:O       | 2:B:24:LEU:HB2     | 2.05                     | 0.57              |
| 3:C:278:ALA:O      | 3:C:282:MET:HB2    | 2.03                     | 0.57              |
| 3:C:348:GLU:CD     | 3:C:349:ILE:HG13   | 2.28                     | 0.57              |
| 3:C:465:PRO:HG2    | 8:I:32:PRO:HB3     | 1.87                     | 0.57              |
| 22:C:1029:CLA:HMA2 | 22:C:1029:CLA:CBA  | 2.25                     | 0.57              |
| 22:C:1029:CLA:CHA  | 22:C:1029:CLA:CGA  | 2.83                     | 0.57              |
| 22:C:1032:CLA:H2   | 22:K:1034:CLA:CMB  | 2.35                     | 0.57              |
| 4:D:110:LEU:H      | 4:D:110:LEU:HD12   | 1.70                     | 0.57              |
| 14:T:11:ALA:O      | 14:T:12:CYS:C      | 2.46                     | 0.57              |
| 2:b:5144:PHE:O     | 2:b:5148:LEU:HB2   | 2.04                     | 0.57              |
| 22:b:6012:CLA:HBD  | 22:b:6012:CLA:HAA1 | 1.86                     | 0.57              |
| 22:b:6014:CLA:C4   | 22:b:6014:CLA:H71  | 2.34                     | 0.57              |
| 22:b:6023:CLA:C3C  | 22:b:6024:CLA:HBC1 | 2.33                     | 0.57              |
| 3:c:5278:ALA:O     | 3:c:5282:MET:HB2   | 2.03                     | 0.57              |
| 3:c:5430:HIS:H     | 3:c:5430:HIS:HD1   | 1.51                     | 0.57              |
| 3:c:5443:TRP:CD1   | 22:c:6032:CLA:HMD3 | 2.40                     | 0.57              |
| 3:c:5457:LYS:HZ1   | 4:d:5228:GLY:HA2   | 1.68                     | 0.57              |
| 4:d:5089:LEU:HB2   | 4:d:5091:LEU:CD1   | 2.35                     | 0.57              |
| 4:d:5193:LEU:O     | 4:d:5193:LEU:HD23  | 2.04                     | 0.57              |
| 9:j:5007:ARG:HG2   | 9:j:5007:ARG:HH11  | 1.69                     | 0.57              |
| 13:o:5041:LEU:HD22 | 13:o:5044:LYS:HD2  | 1.86                     | 0.57              |
| 13:o:5055:ALA:CB   | 13:o:5161:SER:HB3  | 2.30                     | 0.57              |
| 25:t:1046:BCR:H323 | 25:t:1046:BCR:C4   | 2.33                     | 0.57              |
| 18:y:5039:LEU:CD2  | 20:z:5028:ALA:CB   | 2.83                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1023:CLA:CED  | 22:B:1024:CLA:HBB2 | 2.32                     | 0.57              |
| 5:E:20:TRP:HZ2     | 9:J:13:VAL:CG2     | 2.14                     | 0.57              |
| 13:O:184:ASP:O     | 13:O:185:PRO:C     | 2.47                     | 0.57              |
| 16:V:38:LEU:CB     | 16:V:45:ILE:HD11   | 2.33                     | 0.57              |
| 16:V:94:ASN:C      | 16:V:96:GLU:H      | 2.12                     | 0.57              |
| 22:c:6031:CLA:CAD  | 22:c:6033:CLA:H122 | 2.32                     | 0.57              |
| 4:d:5017:ILE:HD12  | 17:x:5041:SER:OG   | 2.04                     | 0.57              |
| 4:d:5055:VAL:HG22  | 4:d:5105:CYS:SG    | 2.45                     | 0.57              |
| 4:d:5109:GLY:C     | 4:d:5111:TRP:N     | 2.62                     | 0.57              |
| 23:d:6039:PHO:O2A  | 23:d:6039:PHO:C4   | 2.53                     | 0.57              |
| 13:o:5079:LYS:HE2  | 13:o:5089:ALA:CB   | 2.33                     | 0.57              |
| 13:o:5132:VAL:CG2  | 13:o:5144:LEU:HD21 | 2.30                     | 0.57              |
| 15:u:5069:GLU:HA   | 15:u:5072:LYS:HE3  | 1.87                     | 0.57              |
| 16:v:5094:ASN:C    | 16:v:5096:GLU:H    | 2.12                     | 0.57              |
| 1:A:288:LEU:HD22   | 3:C:432:VAL:HG23   | 1.87                     | 0.57              |
| 2:B:144:PHE:O      | 2:B:148:LEU:HB2    | 2.04                     | 0.57              |
| 2:B:402:TYR:N      | 2:B:402:TYR:CD1    | 2.73                     | 0.57              |
| 25:B:1047:BCR:H403 | 25:B:1047:BCR:C22  | 2.34                     | 0.57              |
| 3:C:160:ILE:HG21   | 22:C:1033:CLA:H202 | 1.85                     | 0.57              |
| 3:C:299:SER:O      | 3:C:302:TYR:O      | 2.23                     | 0.57              |
| 22:C:1026:CLA:C1B  | 22:C:1028:CLA:HBB2 | 2.35                     | 0.57              |
| 23:D:1039:PHO:O2A  | 23:D:1039:PHO:C4   | 2.53                     | 0.57              |
| 18:Y:39:LEU:CD2    | 20:Z:28:ALA:CB     | 2.83                     | 0.57              |
| 20:Z:58:ASN:C      | 20:Z:60:PHE:H      | 2.13                     | 0.57              |
| 2:b:5327:THR:HG23  | 11:l:5037:ASN:HD22 | 1.69                     | 0.57              |
| 3:c:5121:SER:O     | 3:c:5125:LEU:HD12  | 2.04                     | 0.57              |
| 22:c:6037:CLA:CBC  | 22:c:6037:CLA:CHD  | 2.76                     | 0.57              |
| 4:d:5029:PHE:HE2   | 4:d:5031:GLY:HA3   | 1.69                     | 0.57              |
| 4:d:5188:PHE:HE2   | 4:d:5326:ARG:HA    | 1.70                     | 0.57              |
| 22:d:6004:CLA:C14  | 22:d:6004:CLA:H102 | 2.34                     | 0.57              |
| 22:k:6034:CLA:H102 | 22:k:6034:CLA:C14  | 2.13                     | 0.57              |
| 16:v:5038:LEU:HD12 | 16:v:5095:ILE:CG2  | 2.35                     | 0.57              |
| 20:z:5053:VAL:C    | 20:z:5055:GLY:N    | 2.57                     | 0.57              |
| 1:A:259:ILE:HG23   | 4:D:128:ARG:HH12   | 1.70                     | 0.57              |
| 3:C:49:LEU:HG      | 22:C:1035:CLA:HMA2 | 1.87                     | 0.57              |
| 4:D:188:PHE:HE2    | 4:D:326:ARG:HA     | 1.70                     | 0.57              |
| 9:J:10:LEU:O       | 9:J:13:VAL:HG12    | 2.05                     | 0.57              |
| 11:L:29:LEU:HB2    | 14:T:9:ILE:CG2     | 2.29                     | 0.57              |
| 13:O:44:LYS:HA     | 13:O:72:GLN:CD     | 2.30                     | 0.57              |
| 16:V:38:LEU:HD12   | 16:V:95:ILE:CG2    | 2.35                     | 0.57              |
| 16:V:117:VAL:O     | 16:V:117:VAL:HG12  | 2.05                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:Z:53:VAL:C      | 20:Z:55:GLY:N      | 2.57                     | 0.57              |
| 2:b:5193:TYR:O     | 2:b:5261:ALA:HB2   | 2.04                     | 0.57              |
| 2:b:5258:TYR:CE2   | 29:b:6058:DGD:HG32 | 2.40                     | 0.57              |
| 22:b:6011:CLA:CMD  | 22:b:6014:CLA:CAB  | 2.83                     | 0.57              |
| 3:c:5040:ALA:O     | 3:c:5043:ILE:HG22  | 2.05                     | 0.57              |
| 3:c:5371:GLY:O     | 13:o:5033:TYR:HB2  | 2.04                     | 0.57              |
| 22:c:6025:CLA:HMB2 | 25:c:6054:BCR:C24  | 2.35                     | 0.57              |
| 4:d:5251:ARG:HB3   | 4:d:5251:ARG:NH1   | 2.20                     | 0.57              |
| 6:f:5041:GLN:HE21  | 9:j:5028:PHE:HA    | 1.65                     | 0.57              |
| 18:y:5039:LEU:HD21 | 20:z:5028:ALA:HB3  | 1.86                     | 0.57              |
| 20:z:5055:GLY:HA2  | 25:z:6053:BCR:H313 | 1.82                     | 0.57              |
| 20:z:5058:ASN:C    | 20:z:5060:PHE:H    | 2.13                     | 0.57              |
| 2:B:170:ASP:CB     | 2:B:171:PRO:HD2    | 2.32                     | 0.57              |
| 22:B:1010:CLA:HMD3 | 22:B:1011:CLA:H92  | 1.87                     | 0.57              |
| 29:C:1056:DGD:HB1  | 29:C:1056:DGD:CAB  | 2.30                     | 0.57              |
| 4:D:17:ILE:HD12    | 17:X:41:SER:OG     | 2.04                     | 0.57              |
| 4:D:66:SER:HB3     | 4:D:69:GLU:HG3     | 1.87                     | 0.57              |
| 8:I:24:LEU:O       | 8:I:26:GLY:N       | 2.37                     | 0.57              |
| 18:Y:45:ASN:C      | 18:Y:45:ASN:ND2    | 2.59                     | 0.57              |
| 1:a:5063:ILE:HD13  | 1:a:5063:ILE:H     | 1.69                     | 0.57              |
| 2:b:5418:LYS:O     | 2:b:5419:SER:C     | 2.48                     | 0.57              |
| 4:d:5266:TRP:CD1   | 28:d:6062:MGE:H2D  | 2.39                     | 0.57              |
| 4:d:5326:ARG:HH11  | 4:d:5326:ARG:HG3   | 1.70                     | 0.57              |
| 24:d:6042:PQ9:H241 | 24:d:6042:PQ9:C28  | 2.35                     | 0.57              |
| 5:e:5020:TRP:HZ2   | 9:j:5013:VAL:CG2   | 2.14                     | 0.57              |
| 10:k:5028:ILE:HA   | 10:k:5031:LEU:HD12 | 1.86                     | 0.57              |
| 16:v:5134:THR:H    | 16:v:5137:ASP:HB2  | 1.70                     | 0.57              |
| 1:A:279:ARG:CB     | 4:D:212:ALA:HB2    | 2.31                     | 0.57              |
| 2:B:3:LEU:HD22     | 11:L:8:GLN:CB      | 2.34                     | 0.57              |
| 3:C:75:PHE:CZ      | 3:C:105:VAL:HG11   | 2.37                     | 0.57              |
| 3:C:307:PRO:HB3    | 3:C:358:PHE:HB3    | 1.87                     | 0.57              |
| 4:D:281:MET:HE2    | 4:D:281:MET:N      | 2.20                     | 0.57              |
| 5:E:23:HIS:O       | 5:E:24:SER:C       | 2.47                     | 0.57              |
| 1:a:5192:ILE:CD1   | 1:a:5198:HIS:HB2   | 2.34                     | 0.57              |
| 2:b:5226:TYR:HA    | 2:b:5231:MET:SD    | 2.44                     | 0.57              |
| 2:b:5332:LYS:HG2   | 2:b:5439:SER:HA    | 1.87                     | 0.57              |
| 2:b:5402:TYR:N     | 2:b:5402:TYR:CD1   | 2.73                     | 0.57              |
| 3:c:5266:TRP:CD1   | 3:c:5266:TRP:N     | 2.73                     | 0.57              |
| 3:c:5334:PRO:CA    | 13:o:5179:THR:OG1  | 2.53                     | 0.57              |
| 3:c:5377:LEU:HD13  | 3:c:5377:LEU:O     | 2.05                     | 0.57              |
| 4:d:5222:LEU:HD21  | 4:d:5243:THR:OG1   | 2.04                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k:5028:ILE:O    | 10:k:5031:LEU:HB2  | 2.04                     | 0.57              |
| 16:v:5038:LEU:HD12 | 16:v:5095:ILE:HG21 | 1.87                     | 0.57              |
| 1:A:63:ILE:HD13    | 1:A:63:ILE:H       | 1.69                     | 0.56              |
| 1:A:104:GLU:OE1    | 13:O:99:ARG:HD2    | 2.04                     | 0.56              |
| 1:A:336:ALA:O      | 1:A:337:HIS:C      | 2.48                     | 0.56              |
| 2:B:251:VAL:HG13   | 22:B:1010:CLA:H2   | 1.86                     | 0.56              |
| 2:B:258:TYR:CE2    | 29:B:1058:DGD:HG32 | 2.40                     | 0.56              |
| 2:B:390:TYR:N      | 2:B:390:TYR:CD1    | 2.73                     | 0.56              |
| 3:C:155:ASN:HA     | 3:C:158:THR:CG2    | 2.29                     | 0.56              |
| 22:C:1025:CLA:HMB2 | 25:C:1054:BCR:C24  | 2.35                     | 0.56              |
| 24:D:1042:PQ9:H241 | 24:D:1042:PQ9:C28  | 2.35                     | 0.56              |
| 6:F:40:MET:C       | 6:F:42:PHE:H       | 2.13                     | 0.56              |
| 6:F:45:ARG:HE      | 6:F:45:ARG:CA      | 1.97                     | 0.56              |
| 13:O:172:PHE:CZ    | 13:O:223:ILE:HG23  | 2.40                     | 0.56              |
| 15:U:78:ASN:HB3    | 15:U:82:PHE:CE2    | 2.40                     | 0.56              |
| 16:V:38:LEU:HB2    | 16:V:45:ILE:CG1    | 2.34                     | 0.56              |
| 2:b:5074:SER:C     | 2:b:5076:SER:H     | 2.12                     | 0.56              |
| 22:b:6019:CLA:H91  | 28:b:6060:MGE:H112 | 1.87                     | 0.56              |
| 22:b:6022:CLA:O2A  | 22:b:6022:CLA:CHA  | 2.52                     | 0.56              |
| 22:c:6029:CLA:CHA  | 22:c:6029:CLA:CGA  | 2.83                     | 0.56              |
| 22:c:6031:CLA:CAD  | 22:c:6033:CLA:H161 | 2.34                     | 0.56              |
| 4:d:5185:PHE:CE1   | 4:d:5289:LEU:HD13  | 2.40                     | 0.56              |
| 4:d:5274:VAL:CB    | 4:d:5275:PRO:HD3   | 2.30                     | 0.56              |
| 5:e:5022:ILE:HG23  | 19:n:5018:UNK:HA   | 1.86                     | 0.56              |
| 8:i:5010:ILE:HD13  | 8:i:5010:ILE:H     | 1.70                     | 0.56              |
| 13:o:5168:PHE:N    | 13:o:5225:LEU:O    | 2.37                     | 0.56              |
| 13:o:5184:ASP:O    | 13:o:5185:PRO:C    | 2.47                     | 0.56              |
| 15:u:5043:PRO:CB   | 16:v:5109:ASP:HB2  | 2.35                     | 0.56              |
| 1:A:29:TYR:CG      | 1:A:133:LEU:HD13   | 2.40                     | 0.56              |
| 1:A:200:LEU:HD23   | 29:C:1057:DGD:HBW2 | 1.86                     | 0.56              |
| 2:B:327:THR:HG23   | 11:L:37:ASN:HD22   | 1.69                     | 0.56              |
| 22:B:1019:CLA:H91  | 28:B:1060:MGE:H112 | 1.86                     | 0.56              |
| 22:B:1023:CLA:ND   | 22:B:1024:CLA:CMC  | 2.69                     | 0.56              |
| 3:C:40:ALA:O       | 3:C:43:ILE:HG22    | 2.05                     | 0.56              |
| 4:D:326:ARG:HH11   | 4:D:326:ARG:HG3    | 1.70                     | 0.56              |
| 11:L:4:ASN:HD21    | 11:L:6:ASN:HD22    | 1.53                     | 0.56              |
| 20:Z:10:ALA:O      | 20:Z:14:ILE:HG13   | 2.05                     | 0.56              |
| 20:Z:44:SER:O      | 20:Z:48:ILE:HD13   | 2.05                     | 0.56              |
| 1:a:5111:PRO:O     | 1:a:5112:TYR:C     | 2.48                     | 0.56              |
| 1:a:5167:SER:C     | 1:a:5169:SER:H     | 2.13                     | 0.56              |
| 1:a:5219:VAL:HB    | 4:d:5268:HIS:HB3   | 1.86                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:a:6038:PHO:CHD  | 23:a:6038:PHO:CBC  | 2.81                     | 0.56              |
| 2:b:5009:HIS:CG    | 22:b:6020:CLA:HBB2 | 2.40                     | 0.56              |
| 2:b:5153:PHE:HB2   | 22:b:6014:CLA:HMC3 | 1.87                     | 0.56              |
| 2:b:5390:TYR:N     | 2:b:5390:TYR:CD1   | 2.73                     | 0.56              |
| 22:b:6016:CLA:C2   | 22:h:6017:CLA:H91  | 2.31                     | 0.56              |
| 3:c:5443:TRP:HD1   | 22:c:6032:CLA:HMD3 | 1.68                     | 0.56              |
| 22:c:6026:CLA:C1B  | 22:c:6028:CLA:HBB2 | 2.35                     | 0.56              |
| 13:o:5044:LYS:HA   | 13:o:5072:GLN:CD   | 2.30                     | 0.56              |
| 13:o:5172:PHE:CZ   | 13:o:5223:ILE:HG23 | 2.40                     | 0.56              |
| 15:u:5028:ASN:HD22 | 15:u:5054:PRO:CB   | 2.18                     | 0.56              |
| 18:y:5043:ARG:CG   | 18:y:5044:GLY:N    | 2.66                     | 0.56              |
| 20:z:5050:LEU:O    | 20:z:5054:VAL:HG23 | 2.05                     | 0.56              |
| 1:A:119:PHE:CE2    | 1:A:123:ALA:HB2    | 2.40                     | 0.56              |
| 1:A:123:ALA:O      | 1:A:126:TYR:HB3    | 2.06                     | 0.56              |
| 1:A:128:GLY:C      | 1:A:130:GLN:H      | 2.13                     | 0.56              |
| 2:B:389:LYS:HB3    | 2:B:390:TYR:CD1    | 2.40                     | 0.56              |
| 22:B:1010:CLA:HED3 | 22:B:1011:CLA:HMA2 | 1.86                     | 0.56              |
| 22:B:1016:CLA:O1D  | 22:B:1016:CLA:H2A  | 2.06                     | 0.56              |
| 3:C:33:PHE:N       | 3:C:33:PHE:HD1     | 2.04                     | 0.56              |
| 3:C:135:ARG:HB2    | 20:Z:27:TYR:CD1    | 2.41                     | 0.56              |
| 3:C:156:LYS:O      | 3:C:160:ILE:HD13   | 2.06                     | 0.56              |
| 3:C:443:TRP:CD1    | 22:C:1032:CLA:HMD3 | 2.40                     | 0.56              |
| 22:C:1029:CLA:CHC  | 22:C:1029:CLA:HBB1 | 2.35                     | 0.56              |
| 22:C:1031:CLA:HAA2 | 22:C:1031:CLA:HBD  | 1.88                     | 0.56              |
| 4:D:185:PHE:CE1    | 4:D:289:LEU:HD13   | 2.40                     | 0.56              |
| 4:D:186:GLN:N      | 22:D:1004:CLA:HBC1 | 2.21                     | 0.56              |
| 4:D:251:ARG:HB3    | 4:D:251:ARG:NH1    | 2.20                     | 0.56              |
| 5:E:27:ILE:CB      | 5:E:28:PRO:HD3     | 2.35                     | 0.56              |
| 6:F:37:ILE:HA      | 6:F:40:MET:CE      | 2.36                     | 0.56              |
| 7:H:30:LEU:HD12    | 7:H:33:VAL:CG2     | 2.35                     | 0.56              |
| 7:H:50:ASN:ND2     | 7:H:50:ASN:O       | 2.39                     | 0.56              |
| 25:H:1049:BCR:H401 | 17:X:20:PHE:CZ     | 2.41                     | 0.56              |
| 8:I:10:ILE:H       | 8:I:10:ILE:HD13    | 1.70                     | 0.56              |
| 22:K:1034:CLA:O1D  | 22:K:1034:CLA:CAA  | 2.30                     | 0.56              |
| 11:L:31:PHE:O      | 11:L:32:SER:C      | 2.47                     | 0.56              |
| 12:M:34:LYS:HG3    | 11:l:5009:PRO:HG2  | 1.85                     | 0.56              |
| 13:O:39:THR:OG1    | 13:O:41:LEU:HB2    | 2.05                     | 0.56              |
| 13:O:73:PRO:HA     | 13:O:263:GLY:HA3   | 1.87                     | 0.56              |
| 13:O:82:PRO:HG2    | 13:O:89:ALA:HB2    | 1.86                     | 0.56              |
| 1:a:5029:TYR:CG    | 1:a:5133:LEU:HD13  | 2.40                     | 0.56              |
| 2:b:5103:LEU:HD21  | 22:b:6013:CLA:CMC  | 2.35                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5036:TRP:CE3   | 3:c:5037:ALA:HB2   | 2.41                     | 0.56              |
| 3:c:5127:PHE:O     | 3:c:5127:PHE:HD2   | 1.88                     | 0.56              |
| 3:c:5245:ILE:O     | 3:c:5249:ILE:HD13  | 2.05                     | 0.56              |
| 3:c:5299:SER:O     | 3:c:5302:TYR:O     | 2.23                     | 0.56              |
| 3:c:5334:PRO:HA    | 13:o:5179:THR:HB   | 1.88                     | 0.56              |
| 4:d:5186:GLN:N     | 22:d:6004:CLA:HBC1 | 2.21                     | 0.56              |
| 4:d:5281:MET:HE2   | 4:d:5281:MET:N     | 2.20                     | 0.56              |
| 25:d:6050:BCR:C17  | 28:d:6059:MGE:H102 | 2.35                     | 0.56              |
| 5:e:5052:PRO:HG2   | 9:j:5036:LEU:HD11  | 1.88                     | 0.56              |
| 5:e:5074:GLN:O     | 5:e:5075:GLN:C     | 2.48                     | 0.56              |
| 6:f:5040:MET:C     | 6:f:5042:PHE:H     | 2.13                     | 0.56              |
| 8:i:5031:ASN:HB2   | 8:i:5032:PRO:CD    | 2.31                     | 0.56              |
| 13:o:5082:PRO:HG2  | 13:o:5089:ALA:HB2  | 1.86                     | 0.56              |
| 13:o:5221:GLY:O    | 13:o:5222:GLN:HB2  | 2.06                     | 0.56              |
| 16:v:5102:MET:SD   | 16:v:5138:LEU:HD22 | 2.45                     | 0.56              |
| 20:z:5044:SER:O    | 20:z:5048:ILE:HD13 | 2.05                     | 0.56              |
| 1:A:94:TYR:HE2     | 13:O:99:ARG:NE     | 2.04                     | 0.56              |
| 2:B:5:TRP:CE2      | 28:L:1061:MGE:H2A2 | 2.40                     | 0.56              |
| 22:B:1011:CLA:CMD  | 22:B:1014:CLA:CAB  | 2.83                     | 0.56              |
| 3:C:142:GLU:C      | 3:C:144:SER:N      | 2.63                     | 0.56              |
| 3:C:266:TRP:CD1    | 3:C:266:TRP:N      | 2.73                     | 0.56              |
| 22:C:1026:CLA:HAA1 | 22:C:1026:CLA:HBD  | 1.87                     | 0.56              |
| 4:D:29:PHE:HE2     | 4:D:31:GLY:HA3     | 1.69                     | 0.56              |
| 4:D:261:PHE:CE1    | 4:D:267:LEU:HG     | 2.41                     | 0.56              |
| 22:D:1004:CLA:HHC  | 22:D:1004:CLA:CBB  | 2.21                     | 0.56              |
| 10:K:20:PRO:HB3    | 18:Y:21:GLN:HA     | 1.87                     | 0.56              |
| 13:O:69:LEU:HG     | 13:O:107:ILE:HD12  | 1.87                     | 0.56              |
| 13:O:231:ASP:OD1   | 13:O:234:THR:HG23  | 2.06                     | 0.56              |
| 13:O:241:PHE:CD1   | 13:O:241:PHE:C     | 2.84                     | 0.56              |
| 16:V:45:ILE:H      | 16:V:45:ILE:CD1    | 2.06                     | 0.56              |
| 20:Z:5:PHE:CD1     | 20:Z:57:LEU:HB3    | 2.41                     | 0.56              |
| 1:a:5111:PRO:HG2   | 1:a:5112:TYR:H     | 1.71                     | 0.56              |
| 22:a:6007:CLA:H142 | 8:i:5013:THR:CG2   | 2.36                     | 0.56              |
| 2:b:5127:ARG:CD    | 2:b:5128:THR:HG23  | 2.31                     | 0.56              |
| 2:b:5238:LEU:N     | 22:b:6020:CLA:HMD3 | 2.21                     | 0.56              |
| 29:b:6058:DGD:C6D  | 29:b:6058:DGD:HE5  | 2.35                     | 0.56              |
| 3:c:5332:GLN:HE22  | 13:o:5175:PRO:HG3  | 1.71                     | 0.56              |
| 22:c:6029:CLA:H12  | 25:c:6054:BCR:H323 | 1.87                     | 0.56              |
| 5:e:5023:HIS:O     | 5:e:5024:SER:C     | 2.47                     | 0.56              |
| 13:o:5241:PHE:CD1  | 13:o:5241:PHE:C    | 2.84                     | 0.56              |
| 16:v:5117:VAL:O    | 16:v:5117:VAL:HG12 | 2.05                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:140:ARG:HH21   | 26:A:1063:LHG:C3   | 2.19                     | 0.56              |
| 1:A:167:SER:C      | 1:A:169:SER:N      | 2.60                     | 0.56              |
| 2:B:96:VAL:O       | 2:B:99:ALA:HB3     | 2.04                     | 0.56              |
| 2:B:238:LEU:N      | 22:B:1020:CLA:HMD3 | 2.21                     | 0.56              |
| 2:B:267:LEU:C      | 2:B:268:PHE:CD1    | 2.84                     | 0.56              |
| 2:B:317:ASN:HA     | 2:B:330:MET:CE     | 2.36                     | 0.56              |
| 22:B:1011:CLA:H202 | 7:H:38:PHE:CE2     | 2.41                     | 0.56              |
| 3:C:48:LYS:HD2     | 22:C:1035:CLA:CED  | 2.33                     | 0.56              |
| 3:C:245:ILE:O      | 3:C:249:ILE:HD13   | 2.05                     | 0.56              |
| 3:C:350:ILE:HG21   | 3:C:359:TRP:CB     | 2.28                     | 0.56              |
| 3:C:377:LEU:HD13   | 3:C:377:LEU:O      | 2.05                     | 0.56              |
| 22:C:1029:CLA:H12  | 25:C:1054:BCR:H323 | 1.87                     | 0.56              |
| 22:D:1005:CLA:C12  | 22:D:1005:CLA:H92  | 2.28                     | 0.56              |
| 7:H:38:PHE:HB2     | 25:H:1049:BCR:C10  | 2.34                     | 0.56              |
| 16:V:102:MET:SD    | 16:V:138:LEU:HD22  | 2.45                     | 0.56              |
| 1:a:5123:ALA:O     | 1:a:5126:TYR:HB3   | 2.06                     | 0.56              |
| 1:a:5197:PHE:CE1   | 1:a:5285:PHE:HD2   | 2.18                     | 0.56              |
| 26:a:6063:LHG:H321 | 22:k:6034:CLA:H172 | 1.88                     | 0.56              |
| 22:b:6024:CLA:HAA2 | 22:b:6024:CLA:HBD  | 1.88                     | 0.56              |
| 22:d:6008:CLA:C18  | 22:d:6008:CLA:H141 | 2.19                     | 0.56              |
| 5:e:5027:ILE:CB    | 5:e:5028:PRO:HD3   | 2.35                     | 0.56              |
| 5:e:5056:TYR:C     | 5:e:5057:ALA:O     | 2.48                     | 0.56              |
| 7:h:5038:PHE:O     | 7:h:5039:LEU:C     | 2.49                     | 0.56              |
| 10:k:5021:LEU:HD21 | 18:y:5024:MET:HG2  | 1.86                     | 0.56              |
| 18:y:5025:ILE:CG1  | 18:y:5026:ALA:N    | 2.69                     | 0.56              |
| 1:A:26:ASN:O       | 1:A:27:ARG:C       | 2.48                     | 0.56              |
| 1:A:142:TRP:HH2    | 26:A:1063:LHG:HC5  | 1.71                     | 0.56              |
| 1:A:199:GLN:NE2    | 22:A:1006:CLA:O1D  | 2.39                     | 0.56              |
| 3:C:286:ALA:O      | 3:C:289:PHE:N      | 2.34                     | 0.56              |
| 3:C:334:PRO:CA     | 13:O:179:THR:OG1   | 2.53                     | 0.56              |
| 22:C:1025:CLA:H3A  | 22:C:1025:CLA:CGA  | 2.28                     | 0.56              |
| 22:C:1026:CLA:HBB2 | 22:K:1034:CLA:C1   | 2.36                     | 0.56              |
| 22:C:1031:CLA:OBD  | 22:C:1033:CLA:C16  | 2.48                     | 0.56              |
| 10:K:21:LEU:HD21   | 18:Y:24:MET:HG2    | 1.86                     | 0.56              |
| 15:U:16:LYS:HA     | 15:U:19:THR:HG23   | 1.88                     | 0.56              |
| 16:V:87:LEU:HB2    | 16:V:108:TYR:OH    | 2.06                     | 0.56              |
| 18:Y:43:ARG:NH2    | 18:Y:44:GLY:N      | 2.53                     | 0.56              |
| 1:a:5026:ASN:O     | 1:a:5027:ARG:C     | 2.48                     | 0.56              |
| 1:a:5045:THR:HG23  | 1:a:5046:ILE:H     | 1.68                     | 0.56              |
| 22:b:6010:CLA:HBD  | 22:b:6010:CLA:H11  | 1.81                     | 0.56              |
| 22:b:6023:CLA:ND   | 22:b:6024:CLA:CMC  | 2.69                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5239:TRP:O     | 3:c:5243:ILE:HG13  | 2.04                     | 0.56              |
| 3:c:5268:GLY:C     | 22:c:6033:CLA:HBC1 | 2.30                     | 0.56              |
| 3:c:5425:TRP:O     | 3:c:5428:THR:HG22  | 2.06                     | 0.56              |
| 22:c:6026:CLA:HBD  | 22:c:6026:CLA:HAA1 | 1.87                     | 0.56              |
| 31:f:6040:HEM:HMB2 | 31:f:6040:HEM:CBB  | 2.32                     | 0.56              |
| 25:h:6049:BCR:H401 | 17:x:5020:PHE:CZ   | 2.41                     | 0.56              |
| 9:j:5010:LEU:O     | 9:j:5013:VAL:HG12  | 2.05                     | 0.56              |
| 11:l:5004:ASN:HD21 | 11:l:5006:ASN:HD22 | 1.53                     | 0.56              |
| 20:z:5005:PHE:CD1  | 20:z:5057:LEU:HB3  | 2.41                     | 0.56              |
| 1:A:64:ARG:NH2     | 13:O:98:THR:HG21   | 2.21                     | 0.56              |
| 1:A:279:ARG:NH1    | 23:A:1038:PHO:HMC3 | 2.20                     | 0.56              |
| 22:A:1007:CLA:H142 | 8:I:13:THR:CG2     | 2.36                     | 0.56              |
| 29:B:1058:DGD:C6D  | 29:B:1058:DGD:HE5  | 2.35                     | 0.56              |
| 4:D:55:VAL:HG22    | 4:D:105:CYS:SG     | 2.45                     | 0.56              |
| 6:F:29:PRO:O       | 6:F:32:PHE:N       | 2.39                     | 0.56              |
| 13:O:59:ASP:O      | 13:O:60:SER:CB     | 2.54                     | 0.56              |
| 13:O:69:LEU:HD11   | 13:O:71:LEU:HD21   | 1.88                     | 0.56              |
| 13:O:70:CYS:SG     | 13:O:105:ASP:HB3   | 2.46                     | 0.56              |
| 13:O:221:GLY:O     | 13:O:222:GLN:HB2   | 2.05                     | 0.56              |
| 1:a:5288:LEU:HD22  | 3:c:5432:VAL:HG23  | 1.87                     | 0.56              |
| 2:b:5317:ASN:HA    | 2:b:5330:MET:CE    | 2.36                     | 0.56              |
| 3:c:5033:PHE:N     | 3:c:5033:PHE:HD1   | 2.03                     | 0.56              |
| 3:c:5135:ARG:HB2   | 20:z:5027:TYR:CD1  | 2.41                     | 0.56              |
| 22:c:6026:CLA:HBB2 | 22:k:6034:CLA:C1   | 2.36                     | 0.56              |
| 4:d:5188:PHE:HE2   | 4:d:5326:ARG:CG    | 2.17                     | 0.56              |
| 7:h:5031:MET:HB2   | 22:h:6017:CLA:CAD  | 2.36                     | 0.56              |
| 7:h:5041:PHE:CE1   | 7:h:5045:ILE:HD11  | 2.40                     | 0.56              |
| 25:k:6051:BCR:H331 | 18:y:5028:ILE:HB   | 1.87                     | 0.56              |
| 15:u:5078:ASN:HB3  | 15:u:5082:PHE:CE2  | 2.40                     | 0.56              |
| 1:A:110:GLY:N      | 1:A:111:PRO:HD2    | 2.20                     | 0.56              |
| 2:B:74:SER:HB3     | 2:B:78:TRP:CE2     | 2.41                     | 0.56              |
| 22:B:1023:CLA:H41  | 25:B:1048:BCR:H343 | 1.87                     | 0.56              |
| 3:C:147:PHE:O      | 3:C:156:LYS:HD2    | 2.06                     | 0.56              |
| 3:C:268:GLY:C      | 22:C:1033:CLA:HBC1 | 2.30                     | 0.56              |
| 4:D:58:TRP:CZ3     | 5:E:55:TYR:HB3     | 2.41                     | 0.56              |
| 16:V:134:THR:H     | 16:V:137:ASP:HB2   | 1.70                     | 0.56              |
| 16:V:159:GLY:HA2   | 16:V:163:TYR:CE1   | 2.41                     | 0.56              |
| 18:Y:43:ARG:HD2    | 18:Y:44:GLY:N      | 2.19                     | 0.56              |
| 1:a:5199:GLN:NE2   | 22:a:6006:CLA:O1D  | 2.39                     | 0.56              |
| 1:a:5258:LEU:O     | 1:a:5259:ILE:CD1   | 2.54                     | 0.56              |
| 1:a:5279:ARG:NH2   | 23:a:6038:PHO:CMC  | 2.65                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5181:VAL:HB    | 2:b:5199:VAL:HG21  | 1.87                     | 0.56              |
| 2:b:5390:TYR:N     | 2:b:5390:TYR:HD1   | 2.04                     | 0.56              |
| 2:b:5446:SER:O     | 2:b:5449:GLY:N     | 2.38                     | 0.56              |
| 22:b:6011:CLA:CGA  | 22:b:6011:CLA:C4A  | 2.84                     | 0.56              |
| 4:d:5352:LEU:CD2   | 4:d:5352:LEU:N     | 2.69                     | 0.56              |
| 13:o:5073:PRO:HA   | 13:o:5263:GLY:HA3  | 1.87                     | 0.56              |
| 18:y:5043:ARG:NH2  | 18:y:5044:GLY:N    | 2.53                     | 0.56              |
| 20:z:5010:ALA:O    | 20:z:5014:ILE:HG13 | 2.05                     | 0.56              |
| 1:A:258:LEU:O      | 1:A:259:ILE:CD1    | 2.54                     | 0.56              |
| 1:A:323:ARG:HG3    | 4:D:329:MET:HA     | 1.88                     | 0.56              |
| 2:B:65:PHE:HE2     | 22:B:1012:CLA:CMA  | 1.97                     | 0.56              |
| 2:B:380:ASP:OD1    | 4:D:344:GLU:HG3    | 2.06                     | 0.56              |
| 22:B:1016:CLA:HBD  | 22:B:1016:CLA:HAA1 | 1.86                     | 0.56              |
| 3:C:137:PRO:C      | 3:C:139:THR:H      | 2.12                     | 0.56              |
| 3:C:171:GLY:C      | 3:C:173:LEU:N      | 2.59                     | 0.56              |
| 3:C:248:GLY:O      | 3:C:252:ILE:HB     | 2.06                     | 0.56              |
| 3:C:271:TYR:CE1    | 22:C:1031:CLA:CAC  | 2.83                     | 0.56              |
| 3:C:276:LEU:HG     | 22:C:1032:CLA:HBB1 | 1.88                     | 0.56              |
| 22:C:1033:CLA:C14  | 22:C:1033:CLA:C17  | 2.68                     | 0.56              |
| 13:O:168:PHE:N     | 13:O:225:LEU:O     | 2.37                     | 0.56              |
| 16:V:38:LEU:HD12   | 16:V:95:ILE:HG21   | 1.87                     | 0.56              |
| 1:a:5107:TYR:C     | 1:a:5109:GLY:H     | 2.12                     | 0.56              |
| 1:a:5110:GLY:N     | 1:a:5111:PRO:HD2   | 2.20                     | 0.56              |
| 1:a:5119:PHE:CE2   | 1:a:5123:ALA:HB2   | 2.40                     | 0.56              |
| 2:b:5023:HIS:HD2   | 22:b:6020:CLA:C4A  | 2.19                     | 0.56              |
| 22:b:6011:CLA:H202 | 7:h:5038:PHE:CE2   | 2.41                     | 0.56              |
| 22:b:6023:CLA:HAA2 | 22:b:6023:CLA:HBD  | 1.88                     | 0.56              |
| 3:c:5052:ALA:HB1   | 22:c:6035:CLA:HMB2 | 1.88                     | 0.56              |
| 3:c:5147:PHE:O     | 3:c:5156:LYS:HD2   | 2.06                     | 0.56              |
| 4:d:5261:PHE:CE2   | 4:d:5267:LEU:CA    | 2.89                     | 0.56              |
| 4:d:5342:PRO:O     | 4:d:5345:VAL:HG23  | 2.06                     | 0.56              |
| 22:d:6008:CLA:HBD  | 22:d:6008:CLA:HAA1 | 1.88                     | 0.56              |
| 6:f:5029:PRO:O     | 6:f:5032:PHE:N     | 2.39                     | 0.56              |
| 16:v:5056:LYS:HA   | 16:v:5144:HIS:CE1  | 2.41                     | 0.56              |
| 16:v:5087:LEU:HB2  | 16:v:5108:TYR:OH   | 2.06                     | 0.56              |
| 16:v:5100:ASP:O    | 16:v:5103:LYS:HB2  | 2.05                     | 0.56              |
| 1:A:143:ILE:HG23   | 1:A:144:CYS:N      | 2.21                     | 0.56              |
| 2:B:250:PHE:HB3    | 29:B:1058:DGD:C8B  | 2.36                     | 0.56              |
| 2:B:446:SER:O      | 2:B:449:GLY:N      | 2.38                     | 0.56              |
| 3:C:36:TRP:CE3     | 3:C:37:ALA:HB2     | 2.41                     | 0.56              |
| 7:H:38:PHE:O       | 7:H:39:LEU:C       | 2.49                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5131:TRP:HZ2   | 3:c:5449:ARG:HG2   | 1.71                     | 0.56              |
| 1:a:5259:ILE:HG23  | 4:d:5128:ARG:HH12  | 1.70                     | 0.56              |
| 1:a:5279:ARG:HE    | 23:a:6038:PHO:CMC  | 2.18                     | 0.56              |
| 2:b:5250:PHE:HB3   | 29:b:6058:DGD:C8B  | 2.36                     | 0.56              |
| 22:b:6016:CLA:HAA1 | 22:b:6016:CLA:HBD  | 1.86                     | 0.56              |
| 3:c:5177:ALA:O     | 3:c:5181:PHE:N     | 2.24                     | 0.56              |
| 3:c:5257:PHE:N     | 3:c:5257:PHE:CD1   | 2.73                     | 0.56              |
| 3:c:5276:LEU:HG    | 22:c:6032:CLA:HBB1 | 1.88                     | 0.56              |
| 22:c:6032:CLA:H2   | 22:k:6034:CLA:CMB  | 2.35                     | 0.56              |
| 25:c:6054:BCR:C23  | 25:c:6054:BCR:H402 | 2.31                     | 0.56              |
| 4:d:5033:SER:OG    | 4:d:5128:ARG:CG    | 2.54                     | 0.56              |
| 4:d:5140:PRO:O     | 4:d:5143:ALA:N     | 2.39                     | 0.56              |
| 6:f:5022:ALA:C     | 6:f:5024:HIS:N     | 2.62                     | 0.56              |
| 13:o:5069:LEU:HG   | 13:o:5107:ILE:HD12 | 1.87                     | 0.56              |
| 13:o:5070:CYS:SG   | 13:o:5105:ASP:HB3  | 2.46                     | 0.56              |
| 13:o:5091:PHE:CE1  | 13:o:5260:LYS:HE3  | 2.41                     | 0.56              |
| 14:t:5022:PHE:C    | 14:t:5023:PHE:HD2  | 2.14                     | 0.56              |
| 1:A:110:GLY:N      | 1:A:111:PRO:CD     | 2.69                     | 0.55              |
| 1:A:111:PRO:HG2    | 1:A:112:TYR:H      | 1.71                     | 0.55              |
| 1:A:151:LEU:HD11   | 1:A:155:PHE:HE2    | 1.71                     | 0.55              |
| 2:B:6:TYR:HA       | 22:B:1019:CLA:O2A  | 2.06                     | 0.55              |
| 2:B:97:ALA:O       | 2:B:101:ILE:HG12   | 2.07                     | 0.55              |
| 2:B:103:LEU:HD21   | 22:B:1013:CLA:CMC  | 2.35                     | 0.55              |
| 2:B:107:LEU:O      | 2:B:111:ALA:HB2    | 2.06                     | 0.55              |
| 2:B:332:LYS:HG2    | 2:B:439:SER:HA     | 1.87                     | 0.55              |
| 2:B:418:LYS:O      | 2:B:419:SER:C      | 2.48                     | 0.55              |
| 3:C:199:ILE:CG2    | 3:C:234:VAL:HG11   | 2.33                     | 0.55              |
| 4:D:261:PHE:CE2    | 4:D:267:LEU:CA     | 2.89                     | 0.55              |
| 4:D:274:VAL:CB     | 4:D:275:PRO:HD3    | 2.30                     | 0.55              |
| 14:T:22:PHE:C      | 14:T:23:PHE:HD2    | 2.14                     | 0.55              |
| 15:U:31:ASN:HD22   | 15:U:31:ASN:C      | 2.14                     | 0.55              |
| 20:Z:50:LEU:O      | 20:Z:54:VAL:HG23   | 2.05                     | 0.55              |
| 1:a:5094:TYR:HE2   | 13:o:5099:ARG:NE   | 2.04                     | 0.55              |
| 1:a:5110:GLY:N     | 1:a:5111:PRO:CD    | 2.69                     | 0.55              |
| 1:a:5217:SER:OG    | 4:d:5142:ASN:HA    | 2.06                     | 0.55              |
| 1:a:5228:THR:CG2   | 1:a:5229:GLU:H     | 2.11                     | 0.55              |
| 2:b:5149:LEU:HD13  | 22:b:6012:CLA:C20  | 2.37                     | 0.55              |
| 2:b:5267:LEU:C     | 2:b:5268:PHE:CD1   | 2.84                     | 0.55              |
| 22:b:6016:CLA:H2A  | 22:b:6016:CLA:O1D  | 2.06                     | 0.55              |
| 3:c:5063:TRP:CD1   | 22:c:6028:CLA:HMC1 | 2.41                     | 0.55              |
| 3:c:5248:GLY:O     | 3:c:5252:ILE:HB    | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5053:THR:HG23  | 4:d:5067:TYR:CE2   | 2.41                     | 0.55              |
| 7:h:5006:TRP:NE1   | 7:h:5010:ILE:HD11  | 2.21                     | 0.55              |
| 11:l:5029:LEU:CB   | 14:t:5009:ILE:HG21 | 2.32                     | 0.55              |
| 16:v:5039:ASN:ND2  | 16:v:5040:SER:N    | 2.54                     | 0.55              |
| 26:A:1063:LHG:H321 | 22:K:1034:CLA:H172 | 1.88                     | 0.55              |
| 29:B:1058:DGD:HA31 | 7:H:46:LEU:HD21    | 1.88                     | 0.55              |
| 3:C:60:ILE:HG13    | 22:C:1027:CLA:HMD2 | 1.89                     | 0.55              |
| 22:C:1032:CLA:H2   | 22:K:1034:CLA:HMB1 | 1.87                     | 0.55              |
| 4:D:301:GLN:NE2    | 4:D:313:THR:HG21   | 2.20                     | 0.55              |
| 4:D:342:PRO:O      | 4:D:345:VAL:HG23   | 2.06                     | 0.55              |
| 5:E:78:THR:O       | 5:E:82:GLN:HG2     | 2.05                     | 0.55              |
| 7:H:31:MET:HB2     | 22:H:1017:CLA:CAD  | 2.35                     | 0.55              |
| 13:O:41:LEU:HD22   | 13:O:44:LYS:HD2    | 1.86                     | 0.55              |
| 25:T:6048:BCR:H343 | 22:b:6023:CLA:H41  | 1.88                     | 0.55              |
| 1:a:5151:LEU:HD11  | 1:a:5155:PHE:HE2   | 1.71                     | 0.55              |
| 22:b:6023:CLA:CED  | 22:b:6024:CLA:HBB2 | 2.32                     | 0.55              |
| 25:b:6045:BCR:C34  | 25:b:6047:BCR:H10C | 2.36                     | 0.55              |
| 3:c:5042:LEU:HD21  | 3:c:5048:LYS:CG    | 2.28                     | 0.55              |
| 3:c:5107:ASP:O     | 3:c:5110:PRO:HD2   | 2.06                     | 0.55              |
| 3:c:5156:LYS:O     | 3:c:5160:ILE:HD13  | 2.06                     | 0.55              |
| 3:c:5417:VAL:CG1   | 16:v:5068:VAL:HG11 | 2.25                     | 0.55              |
| 22:c:6029:CLA:CHC  | 22:c:6029:CLA:HBB1 | 2.35                     | 0.55              |
| 4:d:5261:PHE:CE1   | 4:d:5267:LEU:HG    | 2.41                     | 0.55              |
| 6:f:5037:ILE:HA    | 6:f:5040:MET:CE    | 2.36                     | 0.55              |
| 1:A:192:ILE:CG1    | 1:A:293:MET:HE1    | 2.36                     | 0.55              |
| 1:A:202:VAL:HA     | 1:A:205:VAL:CG1    | 2.36                     | 0.55              |
| 22:A:1006:CLA:HAA1 | 22:A:1006:CLA:HBD  | 1.88                     | 0.55              |
| 2:B:122:LEU:HD23   | 7:H:8:GLY:HA2      | 1.86                     | 0.55              |
| 2:B:221:PRO:HA     | 22:H:1017:CLA:HED3 | 1.88                     | 0.55              |
| 3:C:72:LEU:HD23    | 3:C:72:LEU:C       | 2.31                     | 0.55              |
| 4:D:33:SER:OG      | 4:D:128:ARG:CG     | 2.54                     | 0.55              |
| 7:H:41:PHE:CE1     | 7:H:45:ILE:HD11    | 2.40                     | 0.55              |
| 8:I:30:ARG:HH11    | 8:I:30:ARG:HG3     | 1.72                     | 0.55              |
| 25:K:1051:BCR:H331 | 18:Y:28:ILE:HB     | 1.87                     | 0.55              |
| 12:M:15:VAL:O      | 12:M:19:SER:HB2    | 2.07                     | 0.55              |
| 13:O:83:LYS:HE3    | 2:b:5049:ASP:HB3   | 1.88                     | 0.55              |
| 13:O:91:PHE:CE1    | 13:O:260:LYS:HE3   | 2.41                     | 0.55              |
| 20:Z:4:LEU:C       | 20:Z:4:LEU:HD12    | 2.32                     | 0.55              |
| 1:a:5064:ARG:NH2   | 13:o:5098:THR:HG21 | 2.21                     | 0.55              |
| 1:a:5192:ILE:HG12  | 1:a:5293:MET:CE    | 2.36                     | 0.55              |
| 1:a:5192:ILE:CG1   | 1:a:5293:MET:HE1   | 2.36                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5197:PHE:CD1   | 1:a:5285:PHE:HB3   | 2.41                     | 0.55              |
| 2:b:5380:ASP:OD1   | 4:d:5344:GLU:HG3   | 2.06                     | 0.55              |
| 2:b:5384:ARG:HD3   | 15:u:5102:LEU:CD2  | 2.36                     | 0.55              |
| 22:b:6010:CLA:HMD3 | 22:b:6011:CLA:H92  | 1.87                     | 0.55              |
| 25:b:6045:BCR:C23  | 25:b:6045:BCR:C38  | 2.71                     | 0.55              |
| 3:c:5137:PRO:C     | 3:c:5139:THR:H     | 2.12                     | 0.55              |
| 3:c:5286:ALA:O     | 3:c:5289:PHE:N     | 2.34                     | 0.55              |
| 22:c:6031:CLA:HAA2 | 22:c:6031:CLA:HBD  | 1.88                     | 0.55              |
| 22:d:6004:CLA:H201 | 28:d:6059:MGE:C8A  | 2.32                     | 0.55              |
| 7:h:5017:GLU:HB2   | 7:h:5020:LYS:HD3   | 1.88                     | 0.55              |
| 7:h:5050:ASN:ND2   | 7:h:5050:ASN:O     | 2.39                     | 0.55              |
| 10:k:5033:PHE:O    | 10:k:5034:ALA:C    | 2.49                     | 0.55              |
| 13:o:5231:ASP:OD1  | 13:o:5234:THR:HG23 | 2.06                     | 0.55              |
| 16:v:5038:LEU:HB2  | 16:v:5045:ILE:HG13 | 1.88                     | 0.55              |
| 17:x:5029:VAL:O    | 17:x:5033:THR:HB   | 2.07                     | 0.55              |
| 1:A:116:ILE:HD11   | 1:A:158:PHE:O      | 2.06                     | 0.55              |
| 2:B:83:GLU:CG      | 2:B:86:ILE:HD11    | 2.31                     | 0.55              |
| 2:B:278:SER:CB     | 2:B:281:GLN:HG2    | 2.26                     | 0.55              |
| 2:B:454:ALA:C      | 2:B:456:ALA:N      | 2.65                     | 0.55              |
| 22:B:1020:CLA:O2A  | 22:B:1020:CLA:H42  | 2.06                     | 0.55              |
| 3:C:52:ALA:HB1     | 22:C:1035:CLA:HMB2 | 1.88                     | 0.55              |
| 3:C:107:ASP:O      | 3:C:110:PRO:HD2    | 2.06                     | 0.55              |
| 3:C:171:GLY:HA2    | 3:C:174:LEU:CB     | 2.22                     | 0.55              |
| 3:C:291:TRP:HD1    | 3:C:292:PHE:CE2    | 2.25                     | 0.55              |
| 3:C:425:TRP:O      | 3:C:428:THR:HG22   | 2.06                     | 0.55              |
| 4:D:53:THR:HG23    | 4:D:67:TYR:CE2     | 2.41                     | 0.55              |
| 25:D:1050:BCR:C17  | 28:D:1059:MGE:H102 | 2.35                     | 0.55              |
| 5:E:56:TYR:C       | 5:E:57:ALA:O       | 2.48                     | 0.55              |
| 1:a:5040:THR:N     | 22:a:6007:CLA:HBB1 | 2.21                     | 0.55              |
| 22:a:6007:CLA:H112 | 22:a:6007:CLA:C6   | 2.29                     | 0.55              |
| 23:a:6038:PHO:H93  | 22:d:6005:CLA:C18  | 2.28                     | 0.55              |
| 2:b:5030:VAL:O     | 2:b:5031:ALA:C     | 2.50                     | 0.55              |
| 2:b:5033:TRP:CH2   | 2:b:5062:VAL:HG21  | 2.41                     | 0.55              |
| 2:b:5103:LEU:HD11  | 2:b:5107:LEU:CD1   | 2.37                     | 0.55              |
| 22:b:6020:CLA:H42  | 22:b:6020:CLA:O2A  | 2.06                     | 0.55              |
| 3:c:5307:PRO:HB3   | 3:c:5358:PHE:HB3   | 1.87                     | 0.55              |
| 3:c:5429:SER:HB3   | 29:c:6056:DGD:C9A  | 2.34                     | 0.55              |
| 22:c:6031:CLA:CMA  | 22:c:6031:CLA:H2   | 2.36                     | 0.55              |
| 15:u:5042:TYR:CB   | 15:u:5043:PRO:CD   | 2.84                     | 0.55              |
| 1:A:102:LEU:HD12   | 1:A:102:LEU:O      | 2.07                     | 0.55              |
| 1:A:254:TYR:HD1    | 1:A:255:PHE:N      | 2.05                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:303:ASN:HD22   | 1:A:303:ASN:N      | 2.04                     | 0.55              |
| 22:B:1016:CLA:HAB  | 4:D:123:ILE:HG23   | 1.86                     | 0.55              |
| 3:C:84:GLN:O       | 3:C:85:GLY:C       | 2.50                     | 0.55              |
| 3:C:187:ASP:CG     | 3:C:190:ALA:H      | 2.15                     | 0.55              |
| 3:C:431:PHE:O      | 3:C:431:PHE:HD2    | 1.90                     | 0.55              |
| 22:C:1031:CLA:CAD  | 22:C:1033:CLA:H122 | 2.32                     | 0.55              |
| 22:C:1037:CLA:C1B  | 25:Z:1053:BCR:H272 | 2.37                     | 0.55              |
| 4:D:188:PHE:HE2    | 4:D:326:ARG:CG     | 2.17                     | 0.55              |
| 6:F:19:ARG:NH2     | 6:F:20:TRP:HD1     | 2.05                     | 0.55              |
| 25:T:6046:BCR:C35  | 25:b:6047:BCR:C24  | 2.71                     | 0.55              |
| 15:U:43:PRO:CB     | 16:V:109:ASP:HB2   | 2.35                     | 0.55              |
| 1:a:5142:TRP:HH2   | 26:a:6063:LHG:HC5  | 1.71                     | 0.55              |
| 1:a:5279:ARG:CG    | 4:d:5212:ALA:HB2   | 2.36                     | 0.55              |
| 1:a:5332:HIS:HA    | 27:d:6064:IOD:I    | 2.76                     | 0.55              |
| 2:b:5059:GLY:CA    | 2:b:5329:PRO:HB3   | 2.29                     | 0.55              |
| 2:b:5107:LEU:O     | 2:b:5111:ALA:HB2   | 2.06                     | 0.55              |
| 22:b:6019:CLA:HMA2 | 22:b:6020:CLA:HMC1 | 1.88                     | 0.55              |
| 22:b:6022:CLA:C1   | 22:b:6022:CLA:C20  | 2.85                     | 0.55              |
| 29:b:6058:DGD:HA31 | 7:h:5046:LEU:HD21  | 1.88                     | 0.55              |
| 3:c:5059:LEU:HD23  | 10:k:5029:PRO:HA   | 1.89                     | 0.55              |
| 3:c:5291:TRP:HD1   | 3:c:5292:PHE:CE2   | 2.25                     | 0.55              |
| 4:d:5053:THR:HA    | 4:d:5067:TYR:HD2   | 1.69                     | 0.55              |
| 4:d:5058:TRP:CZ3   | 5:e:5055:TYR:HB3   | 2.41                     | 0.55              |
| 4:d:5301:GLN:NE2   | 4:d:5313:THR:HG21  | 2.20                     | 0.55              |
| 9:j:5018:GLY:O     | 9:j:5021:VAL:HG12  | 2.06                     | 0.55              |
| 13:o:5059:ASP:O    | 13:o:5060:SER:CB   | 2.54                     | 0.55              |
| 15:u:5050:VAL:C    | 15:u:5051:LYS:O    | 2.46                     | 0.55              |
| 20:z:5004:LEU:C    | 20:z:5004:LEU:HD12 | 2.32                     | 0.55              |
| 1:A:137:LEU:HB2    | 1:A:139:MET:HE3    | 1.88                     | 0.55              |
| 1:A:192:ILE:HG12   | 1:A:293:MET:CE     | 2.36                     | 0.55              |
| 22:A:1007:CLA:OBD  | 22:A:1007:CLA:CED  | 2.39                     | 0.55              |
| 2:B:125:ASP:HB3    | 2:B:128:THR:HG1    | 1.70                     | 0.55              |
| 2:B:153:PHE:HB2    | 22:B:1014:CLA:HMC3 | 1.87                     | 0.55              |
| 2:B:208:VAL:HG21   | 22:B:1010:CLA:CMC  | 2.37                     | 0.55              |
| 2:B:464:PHE:HB2    | 4:D:280:TRP:CH2    | 2.41                     | 0.55              |
| 3:C:56:HIS:C       | 3:C:56:HIS:HD2     | 2.07                     | 0.55              |
| 3:C:127:PHE:O      | 3:C:130:VAL:HG12   | 2.07                     | 0.55              |
| 3:C:287:THR:CG2    | 3:C:427:ALA:O      | 2.55                     | 0.55              |
| 22:C:1031:CLA:CMA  | 22:C:1031:CLA:H2   | 2.36                     | 0.55              |
| 4:D:48:TRP:CE3     | 4:D:49:LEU:HG      | 2.42                     | 0.55              |
| 4:D:191:TRP:CE3    | 4:D:289:LEU:HD11   | 2.41                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:296:TYR:O      | 4:D:297:ASP:O      | 2.25                     | 0.55              |
| 13:O:167:ASP:HA    | 13:O:225:LEU:O     | 2.07                     | 0.55              |
| 15:U:42:TYR:CB     | 15:U:43:PRO:CD     | 2.84                     | 0.55              |
| 16:V:123:SER:HB2   | 16:V:126:ILE:HD11  | 1.89                     | 0.55              |
| 1:a:5113:GLN:HA    | 1:a:5116:ILE:CG2   | 2.37                     | 0.55              |
| 1:a:5303:ASN:N     | 1:a:5303:ASN:HD22  | 2.04                     | 0.55              |
| 3:c:5199:ILE:HD12  | 3:c:5199:ILE:N     | 2.21                     | 0.55              |
| 3:c:5199:ILE:CG2   | 3:c:5234:VAL:HG11  | 2.33                     | 0.55              |
| 3:c:5443:TRP:CD1   | 22:c:6032:CLA:CMD  | 2.90                     | 0.55              |
| 22:c:6037:CLA:C1B  | 25:z:6053:BCR:H272 | 2.37                     | 0.55              |
| 4:d:5048:TRP:CE3   | 4:d:5049:LEU:HG    | 2.42                     | 0.55              |
| 25:k:6052:BCR:C38  | 25:k:6052:BCR:H372 | 2.23                     | 0.55              |
| 12:m:5015:VAL:O    | 12:m:5019:SER:HB2  | 2.07                     | 0.55              |
| 15:u:5031:ASN:ND2  | 15:u:5032:ILE:N    | 2.48                     | 0.55              |
| 18:y:5043:ARG:HD3  | 20:z:5031:GLN:NE2  | 2.22                     | 0.55              |
| 20:z:5035:ARG:HG3  | 20:z:5036:SER:N    | 2.22                     | 0.55              |
| 1:A:77:ILE:HG12    | 14:T:6:TYR:CD1     | 2.42                     | 0.55              |
| 1:A:167:SER:C      | 1:A:169:SER:H      | 2.13                     | 0.55              |
| 1:A:258:LEU:HA     | 4:D:128:ARG:NH2    | 2.21                     | 0.55              |
| 24:A:1043:PQ9:C45  | 28:D:1059:MGE:C8A  | 2.80                     | 0.55              |
| 26:A:1063:LHG:H292 | 22:C:1032:CLA:C7   | 2.37                     | 0.55              |
| 2:B:68:ARG:HD3     | 22:B:1011:CLA:HED1 | 1.89                     | 0.55              |
| 2:B:354:LEU:C      | 2:B:355:PHE:CD2    | 2.84                     | 0.55              |
| 2:B:384:ARG:HD3    | 15:U:102:LEU:CD2   | 2.36                     | 0.55              |
| 2:B:465:GLY:CA     | 22:B:1019:CLA:HAC1 | 2.37                     | 0.55              |
| 22:B:1022:CLA:C1   | 22:B:1022:CLA:C20  | 2.85                     | 0.55              |
| 22:B:1024:CLA:HAA2 | 22:B:1024:CLA:HBD  | 1.88                     | 0.55              |
| 3:C:127:PHE:O      | 3:C:127:PHE:HD2    | 1.88                     | 0.55              |
| 3:C:334:PRO:HA     | 13:O:179:THR:HB    | 1.88                     | 0.55              |
| 3:C:453:ALA:HB3    | 3:C:455:PHE:CE2    | 2.42                     | 0.55              |
| 4:D:37:LEU:HD13    | 4:D:125:PHE:CA     | 2.37                     | 0.55              |
| 4:D:74:LEU:CD2     | 4:D:175:VAL:HG11   | 2.35                     | 0.55              |
| 24:D:1042:PQ9:H241 | 24:D:1042:PQ9:C27  | 2.37                     | 0.55              |
| 28:D:1059:MGE:H211 | 28:D:1059:MGE:CGB  | 2.37                     | 0.55              |
| 25:H:1049:BCR:H23C | 25:H:1049:BCR:H393 | 1.71                     | 0.55              |
| 9:J:18:GLY:O       | 9:J:21:VAL:HG12    | 2.06                     | 0.55              |
| 25:T:6048:BCR:H342 | 22:b:6014:CLA:H93  | 1.89                     | 0.55              |
| 17:X:29:VAL:O      | 17:X:33:THR:HB     | 2.07                     | 0.55              |
| 1:a:5103:ASP:O     | 1:a:5106:LEU:HB2   | 2.07                     | 0.55              |
| 2:b:5005:TRP:HE3   | 22:b:6019:CLA:H42  | 1.72                     | 0.55              |
| 2:b:5074:SER:HB3   | 2:b:5078:TRP:CE2   | 2.41                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5097:ALA:O     | 2:b:5101:ILE:HG12  | 2.07                     | 0.55              |
| 2:b:5275:TRP:CD1   | 2:b:5318:ASN:ND2   | 2.75                     | 0.55              |
| 2:b:5389:LYS:HB3   | 2:b:5390:TYR:CD1   | 2.40                     | 0.55              |
| 22:b:6009:CLA:HBA1 | 22:b:6009:CLA:O1D  | 1.99                     | 0.55              |
| 3:c:5060:ILE:HG13  | 22:c:6027:CLA:HMD2 | 1.88                     | 0.55              |
| 3:c:5403:SER:O     | 3:c:5406:SER:N     | 2.34                     | 0.55              |
| 22:c:6029:CLA:CBC  | 22:c:6029:CLA:CMC  | 2.84                     | 0.55              |
| 22:c:6035:CLA:H93  | 25:k:6052:BCR:H402 | 1.87                     | 0.55              |
| 4:d:5066:SER:HB3   | 4:d:5069:GLU:HG3   | 1.87                     | 0.55              |
| 28:d:6062:MGE:H222 | 11:l:5022:LEU:HD11 | 1.89                     | 0.55              |
| 8:i:5033:LYS:O     | 8:i:5035:LYS:N     | 2.40                     | 0.55              |
| 13:o:5250:ASP:O    | 13:o:5252:GLY:N    | 2.35                     | 0.55              |
| 15:u:5036:ILE:HG22 | 15:u:5042:TYR:CG   | 2.41                     | 0.55              |
| 16:v:5114:ILE:O    | 16:v:5114:ILE:HG12 | 2.07                     | 0.55              |
| 16:v:5159:GLY:HA2  | 16:v:5163:TYR:CE1  | 2.41                     | 0.55              |
| 1:A:111:PRO:O      | 1:A:112:TYR:C      | 2.48                     | 0.55              |
| 2:B:23:HIS:HD2     | 22:B:1020:CLA:C4A  | 2.19                     | 0.55              |
| 2:B:33:TRP:CH2     | 2:B:62:VAL:HG21    | 2.41                     | 0.55              |
| 2:B:149:LEU:HD13   | 22:B:1012:CLA:C20  | 2.37                     | 0.55              |
| 22:B:1010:CLA:H112 | 22:B:1010:CLA:C17  | 2.36                     | 0.55              |
| 22:B:1020:CLA:C1   | 22:B:1023:CLA:O1A  | 2.55                     | 0.55              |
| 25:B:1045:BCR:C34  | 25:B:1047:BCR:H10C | 2.36                     | 0.55              |
| 3:C:374:GLY:HA2    | 13:O:33:TYR:HD1    | 1.72                     | 0.55              |
| 3:C:414:ILE:HG22   | 3:C:415:ASN:O      | 2.07                     | 0.55              |
| 22:C:1025:CLA:H3A  | 22:C:1025:CLA:H11  | 1.88                     | 0.55              |
| 4:D:210:LEU:HD23   | 4:D:274:VAL:HG21   | 1.89                     | 0.55              |
| 5:E:74:GLN:O       | 5:E:75:GLN:C       | 2.48                     | 0.55              |
| 10:K:40:GLN:HA     | 10:K:40:GLN:OE1    | 2.06                     | 0.55              |
| 11:L:25:LEU:HB3    | 14:T:13:ILE:CG1    | 2.37                     | 0.55              |
| 15:U:84:VAL:HG12   | 15:U:85:THR:N      | 2.21                     | 0.55              |
| 16:V:120:SER:HG    | 16:V:123:SER:HG    | 1.54                     | 0.55              |
| 1:a:5077:ILE:HG12  | 14:t:5006:TYR:CD1  | 2.42                     | 0.55              |
| 1:a:5139:MET:O     | 1:a:5140:ARG:C     | 2.48                     | 0.55              |
| 1:a:5193:LEU:HD11  | 4:d:5182:LEU:HD12  | 1.89                     | 0.55              |
| 1:a:5279:ARG:HG2   | 4:d:5212:ALA:CB    | 2.37                     | 0.55              |
| 1:a:5325:ASN:HD22  | 1:a:5328:MET:CE    | 2.14                     | 0.55              |
| 2:b:5083:GLU:HG2   | 2:b:5086:ILE:CD1   | 2.32                     | 0.55              |
| 2:b:5465:GLY:CA    | 22:b:6019:CLA:HAC1 | 2.37                     | 0.55              |
| 22:b:6015:CLA:H2A  | 22:b:6015:CLA:O1D  | 2.07                     | 0.55              |
| 3:c:5072:LEU:HD23  | 3:c:5072:LEU:C     | 2.31                     | 0.55              |
| 3:c:5127:PHE:O     | 3:c:5130:VAL:HG12  | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5451:ALA:O     | 3:c:5453:ALA:N     | 2.40                     | 0.55              |
| 22:c:6031:CLA:O1A  | 22:c:6033:CLA:C5   | 2.54                     | 0.55              |
| 4:d:5014:TRP:CD1   | 4:d:5015:PHE:N     | 2.75                     | 0.55              |
| 4:d:5230:SER:C     | 4:d:5232:PHE:H     | 2.15                     | 0.55              |
| 24:d:6042:PQ9:H241 | 24:d:6042:PQ9:C27  | 2.37                     | 0.55              |
| 5:e:5078:THR:O     | 5:e:5082:GLN:HG2   | 2.05                     | 0.55              |
| 6:f:5019:ARG:NH2   | 6:f:5020:TRP:HD1   | 2.05                     | 0.55              |
| 13:o:5039:THR:OG1  | 13:o:5041:LEU:HB2  | 2.06                     | 0.55              |
| 13:o:5132:VAL:HG23 | 13:o:5144:LEU:HD23 | 1.86                     | 0.55              |
| 15:u:5084:VAL:HG12 | 15:u:5085:THR:N    | 2.21                     | 0.55              |
| 16:v:5120:SER:HG   | 16:v:5123:SER:HG   | 1.54                     | 0.55              |
| 16:v:5123:SER:HB2  | 16:v:5126:ILE:HD11 | 1.89                     | 0.55              |
| 1:A:40:THR:N       | 22:A:1007:CLA:HBB1 | 2.21                     | 0.55              |
| 1:A:332:HIS:HA     | 27:D:1064:IOD:I    | 2.76                     | 0.55              |
| 2:B:5:TRP:HE3      | 22:B:1019:CLA:H42  | 1.72                     | 0.55              |
| 2:B:181:VAL:HB     | 2:B:199:VAL:HG21   | 1.88                     | 0.55              |
| 25:B:1048:BCR:H392 | 25:B:1048:BCR:C22  | 2.35                     | 0.55              |
| 3:C:56:HIS:HB2     | 3:C:59:LEU:HD13    | 1.89                     | 0.55              |
| 13:O:182:PHE:C     | 13:O:182:PHE:CD2   | 2.85                     | 0.55              |
| 13:O:241:PHE:HD2   | 13:O:265:PHE:HB3   | 1.72                     | 0.55              |
| 1:a:5202:VAL:HA    | 1:a:5205:VAL:CG1   | 2.36                     | 0.55              |
| 1:a:5254:TYR:HD1   | 1:a:5255:PHE:N     | 2.05                     | 0.55              |
| 1:a:5272:HIS:HB3   | 4:d:5218:VAL:CG1   | 2.37                     | 0.55              |
| 22:b:6024:CLA:HBC2 | 22:b:6024:CLA:HMC3 | 1.89                     | 0.55              |
| 3:c:5056:HIS:HB2   | 3:c:5059:LEU:HD13  | 1.89                     | 0.55              |
| 3:c:5151:TRP:CE3   | 3:c:5157:MET:HE1   | 2.42                     | 0.55              |
| 3:c:5160:ILE:HG22  | 22:c:6031:CLA:HMD1 | 1.89                     | 0.55              |
| 3:c:5190:ALA:O     | 3:c:5191:PRO:O     | 2.25                     | 0.55              |
| 3:c:5414:ILE:HG22  | 3:c:5415:ASN:O     | 2.07                     | 0.55              |
| 4:d:5191:TRP:CE3   | 4:d:5289:LEU:HD11  | 2.41                     | 0.55              |
| 11:l:5015:THR:O    | 11:l:5018:TYR:N    | 2.40                     | 0.55              |
| 16:v:5058:LEU:O    | 16:v:5059:PHE:C    | 2.49                     | 0.55              |
| 1:A:322:ASN:HD21   | 3:C:412:THR:HA     | 1.72                     | 0.55              |
| 2:B:69:LEU:HB3     | 22:B:1014:CLA:CMA  | 2.37                     | 0.55              |
| 2:B:400:SER:CB     | 2:B:410:THR:HG22   | 2.38                     | 0.55              |
| 22:B:1012:CLA:HMD2 | 22:B:1020:CLA:C20  | 2.37                     | 0.55              |
| 22:B:1014:CLA:C4   | 22:B:1014:CLA:H71  | 2.34                     | 0.55              |
| 22:B:1020:CLA:H111 | 22:B:1021:CLA:HAB  | 1.89                     | 0.55              |
| 3:C:285:ILE:O      | 3:C:289:PHE:HB2    | 2.07                     | 0.55              |
| 3:C:343:ARG:CG     | 3:C:348:GLU:O      | 2.55                     | 0.55              |
| 3:C:346:THR:HB     | 13:O:38:GLY:CA     | 2.37                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1036:CLA:HBC2 | 22:C:1036:CLA:CMC  | 2.34                     | 0.55              |
| 4:D:194:ASN:O      | 4:D:195:PRO:C      | 2.50                     | 0.55              |
| 4:D:250:ASN:ND2    | 14:T:27:PRO:HG3    | 2.22                     | 0.55              |
| 4:D:352:LEU:CD2    | 4:D:352:LEU:N      | 2.69                     | 0.55              |
| 7:H:17:GLU:HB2     | 7:H:20:LYS:HD3     | 1.89                     | 0.55              |
| 10:K:24:VAL:HG21   | 18:Y:25:ILE:CG2    | 2.26                     | 0.55              |
| 11:L:15:THR:O      | 11:L:18:TYR:N      | 2.40                     | 0.55              |
| 15:U:16:LYS:HZ1    | 15:U:85:THR:HB     | 1.72                     | 0.55              |
| 1:a:5140:ARG:HH21  | 26:a:6063:LHG:C3   | 2.19                     | 0.55              |
| 1:a:5316:THR:C     | 1:a:5318:ALA:H     | 2.15                     | 0.55              |
| 25:a:6044:BCR:H392 | 25:a:6044:BCR:C22  | 2.35                     | 0.55              |
| 2:b:5025:MET:CG    | 25:b:6045:BCR:H391 | 2.37                     | 0.55              |
| 2:b:5026:HIS:HB2   | 22:b:6020:CLA:HMB3 | 1.89                     | 0.55              |
| 3:c:5039:ASN:CB    | 22:c:6032:CLA:HBA1 | 2.35                     | 0.55              |
| 4:d:5032:TRP:HE3   | 4:d:5035:ILE:HD11  | 1.72                     | 0.55              |
| 4:d:5257:PHE:CD2   | 4:d:5257:PHE:O     | 2.60                     | 0.55              |
| 28:d:6059:MGE:H211 | 28:d:6059:MGE:CGB  | 2.37                     | 0.55              |
| 22:k:6034:CLA:H12  | 22:k:6034:CLA:C1D  | 2.37                     | 0.55              |
| 1:A:130:GLN:HG2    | 1:A:144:CYS:HA     | 1.89                     | 0.54              |
| 1:A:139:MET:O      | 1:A:140:ARG:C      | 2.48                     | 0.54              |
| 1:A:183:MET:C      | 22:A:1003:CLA:HBC1 | 2.32                     | 0.54              |
| 1:A:193:LEU:HD11   | 4:D:182:LEU:HD12   | 1.89                     | 0.54              |
| 1:A:197:PHE:CD1    | 1:A:285:PHE:HB3    | 2.41                     | 0.54              |
| 23:A:1038:PHO:H93  | 22:D:1005:CLA:C18  | 2.28                     | 0.54              |
| 2:B:248:ALA:HA     | 22:B:1011:CLA:H51  | 1.90                     | 0.54              |
| 22:B:1012:CLA:HBC3 | 22:B:1012:CLA:CHD  | 2.33                     | 0.54              |
| 22:B:1019:CLA:HHC  | 22:B:1019:CLA:CBB  | 2.34                     | 0.54              |
| 3:C:199:ILE:HD12   | 3:C:199:ILE:N      | 2.21                     | 0.54              |
| 3:C:257:PHE:N      | 3:C:257:PHE:CD1    | 2.73                     | 0.54              |
| 3:C:443:TRP:CD1    | 22:C:1032:CLA:CMD  | 2.90                     | 0.54              |
| 3:C:451:ALA:N      | 3:C:456:GLU:HG2    | 2.22                     | 0.54              |
| 4:D:14:TRP:CD1     | 4:D:15:PHE:N       | 2.75                     | 0.54              |
| 4:D:43:LEU:HD12    | 4:D:117:HIS:CE1    | 2.43                     | 0.54              |
| 4:D:214:HIS:HA     | 4:D:217:THR:HG22   | 1.88                     | 0.54              |
| 22:D:1008:CLA:HAA1 | 22:D:1008:CLA:HBD  | 1.88                     | 0.54              |
| 13:O:242:GLU:HA    | 13:O:261:ILE:O     | 2.08                     | 0.54              |
| 15:U:28:ASN:HD22   | 15:U:54:PRO:CB     | 2.18                     | 0.54              |
| 15:U:42:TYR:O      | 15:U:43:PRO:C      | 2.50                     | 0.54              |
| 16:V:56:LYS:HA     | 16:V:144:HIS:CE1   | 2.41                     | 0.54              |
| 16:V:58:LEU:O      | 16:V:59:PHE:C      | 2.49                     | 0.54              |
| 18:Y:25:ILE:CG1    | 18:Y:26:ALA:N      | 2.69                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5148:SER:O     | 1:a:5149:ALA:C     | 2.50                     | 0.54              |
| 1:a:5183:MET:C     | 22:a:6003:CLA:HBC1 | 2.32                     | 0.54              |
| 2:b:5047:PRO:O     | 2:b:5049:ASP:N     | 2.40                     | 0.54              |
| 2:b:5277:SER:C     | 2:b:5279:TYR:H     | 2.13                     | 0.54              |
| 22:b:6023:CLA:H152 | 22:b:6024:CLA:C1B  | 2.37                     | 0.54              |
| 3:c:5285:ILE:O     | 3:c:5289:PHE:HB2   | 2.07                     | 0.54              |
| 3:c:5431:PHE:HD2   | 3:c:5431:PHE:O     | 1.90                     | 0.54              |
| 4:d:5210:LEU:HD23  | 4:d:5274:VAL:HG21  | 1.89                     | 0.54              |
| 4:d:5250:ASN:ND2   | 14:t:5027:PRO:HG3  | 2.22                     | 0.54              |
| 4:d:5296:TYR:O     | 4:d:5297:ASP:O     | 2.25                     | 0.54              |
| 8:i:5012:VAL:CG1   | 8:i:5013:THR:N     | 2.70                     | 0.54              |
| 10:k:5020:PRO:HB3  | 18:y:5021:GLN:HA   | 1.87                     | 0.54              |
| 13:o:5069:LEU:HD11 | 13:o:5071:LEU:HD21 | 1.88                     | 0.54              |
| 16:v:5159:GLY:HA2  | 16:v:5163:TYR:HE1  | 1.72                     | 0.54              |
| 20:z:5005:PHE:CE1  | 20:z:5054:VAL:HG13 | 2.42                     | 0.54              |
| 1:A:93:PHE:O       | 1:A:95:PRO:CD      | 2.55                     | 0.54              |
| 1:A:272:HIS:CD2    | 4:D:218:VAL:CG2    | 2.86                     | 0.54              |
| 2:B:220:ARG:HD3    | 2:B:221:PRO:CD     | 2.29                     | 0.54              |
| 2:B:346:PHE:CE1    | 2:B:421:ALA:HB2    | 2.43                     | 0.54              |
| 3:C:332:GLN:HE22   | 13:O:175:PRO:HG3   | 1.71                     | 0.54              |
| 22:C:1031:CLA:H142 | 25:C:1054:BCR:C36  | 2.37                     | 0.54              |
| 6:F:42:PHE:O       | 6:F:44:GLN:N       | 2.40                     | 0.54              |
| 7:H:6:TRP:NE1      | 7:H:10:ILE:HD11    | 2.21                     | 0.54              |
| 8:I:27:ASP:N       | 8:I:28:PRO:HD3     | 2.23                     | 0.54              |
| 13:O:86:ARG:HG3    | 13:O:86:ARG:NH1    | 2.22                     | 0.54              |
| 15:U:16:LYS:O      | 15:U:21:TYR:HB3    | 2.06                     | 0.54              |
| 15:U:36:ILE:HG22   | 15:U:42:TYR:CG     | 2.41                     | 0.54              |
| 16:V:38:LEU:HB2    | 16:V:45:ILE:HG13   | 1.88                     | 0.54              |
| 18:Y:32:GLY:O      | 18:Y:35:ILE:CG2    | 2.53                     | 0.54              |
| 18:Y:43:ARG:HD3    | 20:Z:31:GLN:NE2    | 2.22                     | 0.54              |
| 1:a:5022:THR:HG22  | 1:a:5022:THR:O     | 2.08                     | 0.54              |
| 1:a:5093:PHE:O     | 1:a:5095:PRO:CD    | 2.55                     | 0.54              |
| 1:a:5159:LEU:C     | 1:a:5162:PRO:HD2   | 2.33                     | 0.54              |
| 1:a:5335:ASN:ND2   | 13:o:5182:PHE:CZ   | 2.76                     | 0.54              |
| 1:a:5339:PHE:O     | 4:d:5351:ALA:HB1   | 2.07                     | 0.54              |
| 2:b:5158:LEU:HB3   | 2:b:5199:VAL:HG22  | 1.90                     | 0.54              |
| 2:b:5221:PRO:HA    | 22:h:6017:CLA:HED3 | 1.88                     | 0.54              |
| 2:b:5346:PHE:CE1   | 2:b:5421:ALA:HB2   | 2.43                     | 0.54              |
| 22:b:6012:CLA:CHD  | 22:b:6020:CLA:H201 | 2.37                     | 0.54              |
| 22:c:6025:CLA:H3A  | 22:c:6025:CLA:H11  | 1.88                     | 0.54              |
| 4:d:5074:LEU:CD2   | 4:d:5175:VAL:HG11  | 2.35                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5246:MET:O     | 4:d:5249:ALA:HB3   | 2.07                     | 0.54              |
| 4:d:5263:ASN:OD1   | 4:d:5265:ARG:N     | 2.40                     | 0.54              |
| 24:d:6042:PQ9:C23  | 28:l:6061:MGE:H263 | 2.37                     | 0.54              |
| 6:f:5042:PHE:O     | 6:f:5044:GLN:N     | 2.40                     | 0.54              |
| 13:o:5105:ASP:OD1  | 13:o:5106:GLN:HG2  | 2.07                     | 0.54              |
| 1:A:103:ASP:O      | 1:A:106:LEU:HB2    | 2.07                     | 0.54              |
| 1:A:112:TYR:O      | 1:A:116:ILE:HG22   | 2.07                     | 0.54              |
| 1:A:160:ILE:HD13   | 3:C:431:PHE:CZ     | 2.42                     | 0.54              |
| 1:A:187:GLN:O      | 1:A:191:ASN:N      | 2.37                     | 0.54              |
| 1:A:218:LEU:HD11   | 1:A:255:PHE:HB2    | 1.90                     | 0.54              |
| 1:A:335:ASN:ND2    | 13:O:182:PHE:CZ    | 2.76                     | 0.54              |
| 2:B:158:LEU:HB3    | 2:B:199:VAL:HG22   | 1.90                     | 0.54              |
| 2:B:384:ARG:NH1    | 15:U:102:LEU:HD23  | 2.23                     | 0.54              |
| 22:B:1011:CLA:CGA  | 22:B:1011:CLA:C4A  | 2.84                     | 0.54              |
| 25:B:1047:BCR:C24  | 25:t:1046:BCR:C35  | 2.71                     | 0.54              |
| 4:D:246:MET:O      | 4:D:249:ALA:HB3    | 2.07                     | 0.54              |
| 4:D:263:ASN:OD1    | 4:D:265:ARG:N      | 2.40                     | 0.54              |
| 28:D:1062:MGE:H222 | 11:L:22:LEU:HD11   | 1.89                     | 0.54              |
| 8:I:33:LYS:O       | 8:I:35:LYS:N       | 2.40                     | 0.54              |
| 10:K:14:ALA:HB2    | 20:Z:61:VAL:HG22   | 1.90                     | 0.54              |
| 22:K:1034:CLA:H12  | 22:K:1034:CLA:C1D  | 2.37                     | 0.54              |
| 1:a:5116:ILE:HD11  | 1:a:5158:PHE:O     | 2.07                     | 0.54              |
| 1:a:5143:ILE:HG23  | 1:a:5144:CYS:N     | 2.21                     | 0.54              |
| 25:a:6044:BCR:H403 | 25:a:6044:BCR:C22  | 2.36                     | 0.54              |
| 2:b:5006:TYR:HA    | 22:b:6019:CLA:O2A  | 2.06                     | 0.54              |
| 10:k:5035:LEU:HD22 | 25:k:6051:BCR:H352 | 1.88                     | 0.54              |
| 15:u:5016:LYS:O    | 15:u:5021:TYR:HB3  | 2.06                     | 0.54              |
| 1:A:269:ARG:CZ     | 4:D:222:LEU:HD22   | 2.37                     | 0.54              |
| 2:B:21:ALA:HA      | 2:B:24:LEU:HB3     | 1.89                     | 0.54              |
| 2:B:47:PRO:O       | 2:B:49:ASP:N       | 2.40                     | 0.54              |
| 22:B:1015:CLA:HBD  | 22:B:1015:CLA:HAA1 | 1.90                     | 0.54              |
| 22:B:1016:CLA:C3   | 22:H:1017:CLA:C9   | 2.83                     | 0.54              |
| 22:B:1018:CLA:C10  | 22:B:1023:CLA:CBA  | 2.85                     | 0.54              |
| 22:B:1022:CLA:C2D  | 22:B:1022:CLA:C20  | 2.82                     | 0.54              |
| 22:B:1023:CLA:HAA2 | 22:B:1023:CLA:HBD  | 1.88                     | 0.54              |
| 28:B:1060:MGE:C5B  | 4:D:276:VAL:HB     | 2.37                     | 0.54              |
| 3:C:63:TRP:CD1     | 22:C:1028:CLA:HMC1 | 2.41                     | 0.54              |
| 5:E:52:PRO:HG2     | 9:J:36:LEU:HD11    | 1.88                     | 0.54              |
| 8:I:12:VAL:CG1     | 8:I:13:THR:N       | 2.70                     | 0.54              |
| 10:K:39:VAL:HG12   | 10:K:40:GLN:N      | 2.21                     | 0.54              |
| 12:M:34:LYS:HD2    | 12:m:5032:GLN:NE2  | 2.22                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:O:63:THR:HG23   | 13:O:271:PRO:O     | 2.08                     | 0.54              |
| 20:Z:35:ARG:HG3    | 20:Z:36:SER:N      | 2.22                     | 0.54              |
| 1:a:5172:MET:SD    | 1:a:5179:THR:HG22  | 2.47                     | 0.54              |
| 1:a:5267:ASN:O     | 1:a:5270:SER:N     | 2.41                     | 0.54              |
| 1:a:5269:ARG:CZ    | 4:d:5222:LEU:HD22  | 2.37                     | 0.54              |
| 1:a:5296:ASN:HB2   | 3:c:5400:PRO:O     | 2.07                     | 0.54              |
| 2:b:5233:ASN:O     | 2:b:5236:THR:HG22  | 2.07                     | 0.54              |
| 2:b:5454:ALA:C     | 2:b:5456:ALA:N     | 2.65                     | 0.54              |
| 2:b:5464:PHE:HB2   | 4:d:5280:TRP:CH2   | 2.41                     | 0.54              |
| 22:b:6016:CLA:C3   | 22:h:6017:CLA:C9   | 2.83                     | 0.54              |
| 22:b:6018:CLA:H2   | 22:b:6018:CLA:H71  | 1.89                     | 0.54              |
| 22:b:6020:CLA:H111 | 22:b:6021:CLA:HAB  | 1.89                     | 0.54              |
| 3:c:5343:ARG:CG    | 3:c:5348:GLU:O     | 2.55                     | 0.54              |
| 22:c:6032:CLA:H161 | 29:c:6056:DGD:CDB  | 2.37                     | 0.54              |
| 4:d:5043:LEU:HD12  | 4:d:5117:HIS:CE1   | 2.43                     | 0.54              |
| 4:d:5097:ALA:O     | 5:e:5073:LYS:HE2   | 2.08                     | 0.54              |
| 9:j:5020:GLY:HA2   | 9:j:5023:VAL:HG12  | 1.90                     | 0.54              |
| 10:k:5014:ALA:HB2  | 20:z:5061:VAL:HG22 | 1.90                     | 0.54              |
| 11:l:5025:LEU:HB3  | 14:t:5013:ILE:CG1  | 2.37                     | 0.54              |
| 13:o:5079:LYS:HE2  | 13:o:5089:ALA:HB1  | 1.90                     | 0.54              |
| 13:o:5167:ASP:HA   | 13:o:5225:LEU:O    | 2.07                     | 0.54              |
| 15:u:5064:ILE:HG22 | 15:u:5067:LEU:HG   | 1.89                     | 0.54              |
| 1:A:138:GLY:HA2    | 3:C:455:PHE:CE2    | 2.43                     | 0.54              |
| 1:A:217:SER:OG     | 4:D:142:ASN:HA     | 2.06                     | 0.54              |
| 2:B:26:HIS:HB2     | 22:B:1020:CLA:HMB3 | 1.89                     | 0.54              |
| 2:B:233:ASN:O      | 2:B:236:THR:HG22   | 2.08                     | 0.54              |
| 2:B:275:TRP:CD1    | 2:B:318:ASN:ND2    | 2.75                     | 0.54              |
| 2:B:277:SER:C      | 2:B:279:TYR:H      | 2.13                     | 0.54              |
| 2:B:292:LEU:C      | 2:B:294:SER:H      | 2.15                     | 0.54              |
| 3:C:369:LEU:HD13   | 3:C:380:ILE:CD1    | 2.37                     | 0.54              |
| 4:D:109:GLY:C      | 4:D:111:TRP:N      | 2.62                     | 0.54              |
| 7:H:28:THR:O       | 7:H:31:MET:HB3     | 2.08                     | 0.54              |
| 13:O:125:ASP:CG    | 13:O:126:GLY:N     | 2.66                     | 0.54              |
| 15:U:76:ARG:O      | 15:U:79:LEU:HB2    | 2.08                     | 0.54              |
| 15:U:94:GLY:O      | 15:U:95:GLY:C      | 2.51                     | 0.54              |
| 1:a:5090:GLY:HA2   | 1:a:5167:SER:CB    | 2.38                     | 0.54              |
| 1:a:5102:LEU:HD12  | 1:a:5102:LEU:O     | 2.07                     | 0.54              |
| 1:a:5112:TYR:O     | 1:a:5116:ILE:HG22  | 2.07                     | 0.54              |
| 1:a:5128:GLY:C     | 1:a:5130:GLN:H     | 2.13                     | 0.54              |
| 1:a:5160:ILE:HD13  | 3:c:5431:PHE:CZ    | 2.42                     | 0.54              |
| 1:a:5258:LEU:HA    | 4:d:5128:ARG:HH21  | 1.72                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:a:6007:CLA:HAB  | 8:i:5015:PHE:CD2   | 2.43                     | 0.54              |
| 2:b:5005:TRP:CE2   | 28:l:6061:MGE:H2A2 | 2.40                     | 0.54              |
| 2:b:5208:VAL:HG21  | 22:b:6010:CLA:CMC  | 2.37                     | 0.54              |
| 2:b:5275:TRP:CD1   | 2:b:5318:ASN:HD22  | 2.25                     | 0.54              |
| 2:b:5292:LEU:C     | 2:b:5294:SER:H     | 2.15                     | 0.54              |
| 2:b:5453:PHE:O     | 2:b:5456:ALA:HB3   | 2.08                     | 0.54              |
| 22:b:6022:CLA:C2D  | 22:b:6022:CLA:C20  | 2.82                     | 0.54              |
| 28:b:6060:MGE:C5B  | 4:d:5276:VAL:HB    | 2.37                     | 0.54              |
| 3:c:5119:LEU:HD11  | 25:k:6052:BCR:H343 | 1.90                     | 0.54              |
| 3:c:5315:MET:HE1   | 3:c:5380:ILE:HD11  | 1.89                     | 0.54              |
| 4:d:5054:PHE:HB3   | 5:e:5047:PHE:CD1   | 2.41                     | 0.54              |
| 7:h:5056:ASP:C     | 7:h:5058:VAL:N     | 2.63                     | 0.54              |
| 13:o:5063:THR:HG23 | 13:o:5271:PRO:O    | 2.08                     | 0.54              |
| 13:o:5182:PHE:C    | 13:o:5182:PHE:CD2  | 2.85                     | 0.54              |
| 20:z:5001:MET:SD   | 20:z:5004:LEU:HD23 | 2.48                     | 0.54              |
| 1:A:22:THR:HG22    | 1:A:22:THR:O       | 2.07                     | 0.54              |
| 1:A:113:GLN:HA     | 1:A:116:ILE:CG2    | 2.37                     | 0.54              |
| 1:A:159:LEU:C      | 1:A:162:PRO:HD2    | 2.33                     | 0.54              |
| 22:A:1006:CLA:CB   | 22:A:1006:CLA:CHD  | 2.74                     | 0.54              |
| 22:A:1006:CLA:C17  | 25:D:1050:BCR:C28  | 2.70                     | 0.54              |
| 2:B:12:LEU:H       | 2:B:12:LEU:CD1     | 2.15                     | 0.54              |
| 2:B:468:TRP:HE3    | 4:D:144:ILE:HD13   | 1.73                     | 0.54              |
| 22:B:1016:CLA:C17  | 22:D:1008:CLA:HMA1 | 2.34                     | 0.54              |
| 3:C:450:ALA:HB1    | 3:C:456:GLU:HB3    | 1.90                     | 0.54              |
| 22:C:1031:CLA:O1A  | 22:C:1033:CLA:C5   | 2.54                     | 0.54              |
| 22:C:1035:CLA:HBB2 | 22:K:1034:CLA:CMA  | 2.31                     | 0.54              |
| 4:D:54:PHE:HB3     | 5:E:47:PHE:CD1     | 2.41                     | 0.54              |
| 4:D:139:ARG:NH1    | 4:D:265:ARG:HH21   | 1.94                     | 0.54              |
| 4:D:140:PRO:O      | 4:D:143:ALA:N      | 2.39                     | 0.54              |
| 4:D:230:SER:C      | 4:D:232:PHE:H      | 2.15                     | 0.54              |
| 4:D:257:PHE:CD2    | 4:D:257:PHE:O      | 2.60                     | 0.54              |
| 15:U:64:ILE:HG22   | 15:U:67:LEU:HG     | 1.89                     | 0.54              |
| 18:Y:42:ARG:HB2    | 18:Y:43:ARG:HH11   | 1.70                     | 0.54              |
| 1:a:5076:ASN:HD21  | 11:l:5033:SER:C    | 2.15                     | 0.54              |
| 1:a:5258:LEU:HA    | 4:d:5128:ARG:NH2   | 2.21                     | 0.54              |
| 1:a:5270:SER:HB2   | 26:a:6063:LHG:H142 | 1.90                     | 0.54              |
| 1:a:5323:ARG:HG3   | 4:d:5329:MET:HA    | 1.89                     | 0.54              |
| 2:b:5137:LYS:NZ    | 7:h:5014:LEU:O     | 2.41                     | 0.54              |
| 2:b:5169:SER:CB    | 2:b:5176:GLY:HA2   | 2.17                     | 0.54              |
| 22:b:6011:CLA:C2D  | 22:b:6013:CLA:C3   | 2.86                     | 0.54              |
| 3:c:5187:ASP:CG    | 3:c:5190:ALA:H     | 2.15                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5058:TRP:CH2   | 5:e:5055:TYR:HB3   | 2.43                     | 0.54              |
| 4:d:5139:ARG:NH1   | 4:d:5265:ARG:HH21  | 1.94                     | 0.54              |
| 4:d:5276:VAL:HG23  | 4:d:5277:THR:N     | 2.23                     | 0.54              |
| 7:h:5031:MET:HB2   | 22:h:6017:CLA:C3D  | 2.38                     | 0.54              |
| 10:k:5014:ALA:H    | 20:z:5062:VAL:HG11 | 1.73                     | 0.54              |
| 1:A:80:GLY:O       | 1:A:81:ALA:HB2     | 2.07                     | 0.54              |
| 2:B:257:TRP:CE3    | 4:D:291:LEU:HD22   | 2.43                     | 0.54              |
| 2:B:390:TYR:N      | 2:B:390:TYR:HD1    | 2.04                     | 0.54              |
| 22:B:1019:CLA:HBB1 | 22:B:1019:CLA:CHC  | 2.37                     | 0.54              |
| 22:B:1019:CLA:HMA2 | 22:B:1020:CLA:HMC1 | 1.88                     | 0.54              |
| 3:C:315:MET:HE1    | 3:C:380:ILE:HD11   | 1.89                     | 0.54              |
| 3:C:415:ASN:HB3    | 29:C:1057:DGD:O2E  | 2.08                     | 0.54              |
| 22:C:1029:CLA:CBC  | 22:C:1029:CLA:CMC  | 2.84                     | 0.54              |
| 4:D:201:VAL:HG23   | 22:D:1004:CLA:CMB  | 2.19                     | 0.54              |
| 4:D:276:VAL:HG23   | 4:D:277:THR:N      | 2.23                     | 0.54              |
| 24:D:1042:PQ9:C24  | 24:D:1042:PQ9:H292 | 2.37                     | 0.54              |
| 5:E:10:PHE:O       | 5:E:11:SER:C       | 2.51                     | 0.54              |
| 13:O:100:GLU:C     | 13:O:102:THR:H     | 2.16                     | 0.54              |
| 16:V:138:LEU:O     | 16:V:139:VAL:C     | 2.50                     | 0.54              |
| 1:a:5080:GLY:O     | 1:a:5081:ALA:HB2   | 2.07                     | 0.54              |
| 2:b:5325:PHE:O     | 2:b:5327:THR:N     | 2.37                     | 0.54              |
| 3:c:5165:LEU:HD22  | 22:c:6030:CLA:HMC2 | 1.90                     | 0.54              |
| 22:c:6031:CLA:HMA2 | 22:c:6031:CLA:C1   | 2.38                     | 0.54              |
| 4:d:5055:VAL:O     | 4:d:5066:SER:HB2   | 2.08                     | 0.54              |
| 5:e:5034:GLY:HA3   | 6:f:5032:PHE:O     | 2.08                     | 0.54              |
| 7:h:5028:THR:O     | 7:h:5031:MET:HB3   | 2.08                     | 0.54              |
| 15:u:5016:LYS:HA   | 15:u:5019:THR:HG23 | 1.88                     | 0.54              |
| 15:u:5082:PHE:CD2  | 15:u:5082:PHE:N    | 2.76                     | 0.54              |
| 1:A:58:VAL:HB      | 1:A:83:VAL:HG21    | 1.90                     | 0.54              |
| 1:A:223:LEU:O      | 1:A:224:ILE:CB     | 2.41                     | 0.54              |
| 2:B:137:LYS:NZ     | 7:H:14:LEU:O       | 2.41                     | 0.54              |
| 22:B:1023:CLA:H152 | 22:B:1024:CLA:C1B  | 2.37                     | 0.54              |
| 22:B:1024:CLA:HBC2 | 22:B:1024:CLA:HMC3 | 1.89                     | 0.54              |
| 25:B:1047:BCR:H14C | 25:t:1046:BCR:H391 | 1.90                     | 0.54              |
| 3:C:190:ALA:O      | 3:C:191:PRO:O      | 2.25                     | 0.54              |
| 9:J:20:GLY:HA2     | 9:J:23:VAL:HG12    | 1.89                     | 0.54              |
| 12:M:9:ILE:HG23    | 12:M:13:LEU:HD23   | 1.89                     | 0.54              |
| 13:O:85:LYS:CB     | 2:b:5307:GLU:OE2   | 2.50                     | 0.54              |
| 13:O:105:ASP:OD1   | 13:O:106:GLN:HG2   | 2.07                     | 0.54              |
| 16:V:68:VAL:HG13   | 16:V:73:LYS:HE3    | 1.90                     | 0.54              |
| 1:a:5283:VAL:HG21  | 23:a:6038:PHO:HMC3 | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:a:6006:CLA:C17  | 25:d:6050:BCR:C28  | 2.70                     | 0.54              |
| 2:b:5158:LEU:HB2   | 2:b:5199:VAL:HG13  | 1.90                     | 0.54              |
| 2:b:5460:LEU:O     | 4:d:5280:TRP:HZ3   | 1.90                     | 0.54              |
| 2:b:5463:PHE:CE1   | 22:b:6016:CLA:CBB  | 2.89                     | 0.54              |
| 22:b:6021:CLA:CMD  | 22:b:6022:CLA:HBB2 | 2.33                     | 0.54              |
| 25:b:6047:BCR:H392 | 25:b:6047:BCR:C22  | 2.35                     | 0.54              |
| 3:c:5059:LEU:HD21  | 10:k:5032:PHE:CD1  | 2.42                     | 0.54              |
| 3:c:5140:LEU:HD21  | 3:c:5146:PHE:CE1   | 2.29                     | 0.54              |
| 3:c:5287:THR:CG2   | 3:c:5427:ALA:O     | 2.55                     | 0.54              |
| 3:c:5374:GLY:HA2   | 13:o:5033:TYR:HD1  | 1.72                     | 0.54              |
| 3:c:5415:ASN:HB3   | 29:c:6057:DGD:O2E  | 2.07                     | 0.54              |
| 29:c:6056:DGD:C6D  | 29:c:6056:DGD:C4E  | 2.86                     | 0.54              |
| 4:d:5194:ASN:O     | 4:d:5195:PRO:C     | 2.50                     | 0.54              |
| 6:f:5040:MET:CB    | 6:f:5043:ILE:HD11  | 2.38                     | 0.54              |
| 8:i:5010:ILE:H     | 8:i:5010:ILE:CD1   | 2.20                     | 0.54              |
| 10:k:5032:PHE:CE1  | 25:k:6052:BCR:H372 | 2.42                     | 0.54              |
| 12:m:5009:ILE:HG23 | 12:m:5013:LEU:HD23 | 1.89                     | 0.54              |
| 13:o:5242:GLU:HA   | 13:o:5261:ILE:O    | 2.08                     | 0.54              |
| 15:u:5094:GLY:O    | 15:u:5095:GLY:C    | 2.51                     | 0.54              |
| 1:A:116:ILE:CG2    | 1:A:117:PHE:H      | 2.19                     | 0.54              |
| 1:A:180:PHE:CE1    | 4:D:192:THR:O      | 2.61                     | 0.54              |
| 1:A:267:ASN:HB3    | 1:A:270:SER:HG     | 1.71                     | 0.54              |
| 1:A:271:LEU:O      | 1:A:272:HIS:C      | 2.49                     | 0.54              |
| 1:A:296:ASN:HB2    | 3:C:400:PRO:O      | 2.07                     | 0.54              |
| 1:A:307:ILE:HG22   | 1:A:308:ASP:N      | 2.23                     | 0.54              |
| 1:A:315:ASN:O      | 4:D:63:LEU:CD2     | 2.56                     | 0.54              |
| 22:A:1003:CLA:HED2 | 22:A:1003:CLA:CBA  | 2.33                     | 0.54              |
| 2:B:383:PHE:O      | 13:O:192:SER:HA    | 2.08                     | 0.54              |
| 22:B:1015:CLA:O1D  | 22:B:1015:CLA:H2A  | 2.07                     | 0.54              |
| 25:B:1048:BCR:H403 | 25:B:1048:BCR:C22  | 2.34                     | 0.54              |
| 3:C:59:LEU:HD23    | 10:K:29:PRO:HA     | 1.89                     | 0.54              |
| 3:C:322:GLN:HE22   | 3:C:381:LYS:HA     | 1.73                     | 0.54              |
| 4:D:259:ILE:HG22   | 4:D:260:ALA:N      | 2.23                     | 0.54              |
| 9:J:10:LEU:HD13    | 9:J:10:LEU:N       | 2.14                     | 0.54              |
| 13:O:132:VAL:HG23  | 13:O:144:LEU:HD23  | 1.86                     | 0.54              |
| 1:a:5181:ASN:HD22  | 4:d:5314:PHE:HD2   | 1.56                     | 0.54              |
| 1:a:5184:ILE:CG1   | 4:d:5186:GLN:NE2   | 2.66                     | 0.54              |
| 22:a:6006:CLA:CAB  | 22:d:6004:CLA:H51  | 2.37                     | 0.54              |
| 22:a:6006:CLA:HBD  | 22:a:6006:CLA:HAA1 | 1.88                     | 0.54              |
| 2:b:5069:LEU:HB3   | 22:b:6014:CLA:CMA  | 2.37                     | 0.54              |
| 2:b:5306:PRO:HG2   | 2:b:5309:LEU:HB3   | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5384:ARG:NH1   | 15:u:5102:LEU:HD23 | 2.23                     | 0.54              |
| 22:b:6022:CLA:OBD  | 22:b:6022:CLA:CED  | 2.55                     | 0.54              |
| 22:b:6023:CLA:O1D  | 22:b:6024:CLA:CBB  | 2.56                     | 0.54              |
| 3:c:5084:GLN:O     | 3:c:5085:GLY:C     | 2.50                     | 0.54              |
| 3:c:5142:GLU:C     | 3:c:5144:SER:N     | 2.63                     | 0.54              |
| 3:c:5209:ILE:HD13  | 3:c:5236:GLY:HA2   | 1.90                     | 0.54              |
| 3:c:5346:THR:HB    | 13:o:5038:GLY:CA   | 2.36                     | 0.54              |
| 22:c:6026:CLA:C12  | 22:c:6026:CLA:H93  | 2.38                     | 0.54              |
| 4:d:5221:THR:O     | 4:d:5221:THR:HG22  | 2.08                     | 0.54              |
| 6:f:5034:LEU:HD12  | 9:j:5024:ILE:HD13  | 1.90                     | 0.54              |
| 8:i:5027:ASP:N     | 8:i:5028:PRO:HD3   | 2.23                     | 0.54              |
| 11:l:5014:ARG:O    | 11:l:5018:TYR:CD2  | 2.61                     | 0.54              |
| 1:A:64:ARG:CZ      | 13:O:98:THR:HG21   | 2.38                     | 0.54              |
| 1:A:131:TRP:HZ2    | 3:C:449:ARG:HG2    | 1.71                     | 0.54              |
| 22:A:1007:CLA:HAB  | 8:I:15:PHE:CD2     | 2.43                     | 0.54              |
| 2:B:237:VAL:HG13   | 22:B:1018:CLA:C1D  | 2.38                     | 0.54              |
| 3:C:135:ARG:NH1    | 20:Z:33:TRP:CE3    | 2.76                     | 0.54              |
| 3:C:137:PRO:C      | 3:C:139:THR:N      | 2.66                     | 0.54              |
| 4:D:55:VAL:O       | 4:D:66:SER:HB2     | 2.08                     | 0.54              |
| 4:D:97:ALA:O       | 5:E:73:LYS:HE2     | 2.08                     | 0.54              |
| 4:D:221:THR:O      | 4:D:221:THR:HG22   | 2.08                     | 0.54              |
| 4:D:251:ARG:HB3    | 4:D:251:ARG:HH11   | 1.73                     | 0.54              |
| 5:E:34:GLY:HA3     | 6:F:32:PHE:O       | 2.08                     | 0.54              |
| 15:U:82:PHE:CD2    | 15:U:82:PHE:N      | 2.76                     | 0.54              |
| 1:a:5322:ASN:HD21  | 3:c:5412:THR:HA    | 1.72                     | 0.54              |
| 22:a:6007:CLA:HAC1 | 25:a:6044:BCR:C15  | 2.38                     | 0.54              |
| 2:b:5045:PHE:HA    | 2:b:5058:GLN:NE2   | 2.23                     | 0.54              |
| 2:b:5237:VAL:HG13  | 22:b:6018:CLA:C1D  | 2.38                     | 0.54              |
| 2:b:5283:GLU:CG    | 2:b:5286:ARG:HH12  | 2.21                     | 0.54              |
| 22:b:6011:CLA:C9   | 22:b:6011:CLA:CBB  | 2.86                     | 0.54              |
| 22:b:6022:CLA:C1   | 22:b:6022:CLA:H203 | 2.38                     | 0.54              |
| 3:c:5435:PHE:O     | 3:c:5438:LEU:N     | 2.41                     | 0.54              |
| 3:c:5465:PRO:CG    | 8:i:5032:PRO:HB3   | 2.38                     | 0.54              |
| 22:c:6025:CLA:CAD  | 22:c:6025:CLA:CED  | 2.86                     | 0.54              |
| 4:d:5037:LEU:HD13  | 4:d:5125:PHE:CA    | 2.37                     | 0.54              |
| 4:d:5209:LEU:HD23  | 4:d:5209:LEU:C     | 2.33                     | 0.54              |
| 13:o:5092:VAL:HG11 | 13:o:5137:ALA:HB2  | 1.90                     | 0.54              |
| 14:t:5012:CYS:HA   | 27:t:6066:IOD:I    | 2.78                     | 0.54              |
| 17:x:5043:ILE:O    | 17:x:5043:ILE:CG2  | 2.52                     | 0.54              |
| 1:A:267:ASN:O      | 1:A:270:SER:N      | 2.41                     | 0.53              |
| 1:A:336:ALA:O      | 1:A:338:ASN:N      | 2.41                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:339:PHE:HB2    | 27:A:1065:IOD:I    | 2.78                     | 0.53              |
| 25:A:1044:BCR:H403 | 25:A:1044:BCR:C22  | 2.36                     | 0.53              |
| 2:B:19:LEU:HG      | 2:B:23:HIS:CE1     | 2.43                     | 0.53              |
| 2:B:275:TRP:CD1    | 2:B:318:ASN:HD22   | 2.25                     | 0.53              |
| 2:B:394:GLN:OE1    | 15:U:17:LEU:HD21   | 2.08                     | 0.53              |
| 22:B:1011:CLA:C2D  | 22:B:1013:CLA:C3   | 2.86                     | 0.53              |
| 22:B:1021:CLA:CMD  | 22:B:1022:CLA:HBB2 | 2.32                     | 0.53              |
| 22:B:1023:CLA:O1D  | 22:B:1024:CLA:CBB  | 2.56                     | 0.53              |
| 3:C:117:VAL:HG21   | 22:C:1027:CLA:H43  | 1.90                     | 0.53              |
| 3:C:429:SER:HB3    | 29:C:1056:DGD:C9A  | 2.34                     | 0.53              |
| 3:C:435:PHE:O      | 3:C:438:LEU:N      | 2.41                     | 0.53              |
| 3:C:457:LYS:HZ1    | 4:D:228:GLY:HA2    | 1.69                     | 0.53              |
| 29:C:1056:DGD:C6D  | 29:C:1056:DGD:C4E  | 2.86                     | 0.53              |
| 4:D:58:TRP:CH2     | 5:E:55:TYR:HB3     | 2.43                     | 0.53              |
| 4:D:161:PRO:HB3    | 4:D:170:ALA:HB2    | 1.90                     | 0.53              |
| 24:D:1042:PQ9:C23  | 28:L:1061:MGE:H263 | 2.37                     | 0.53              |
| 9:J:30:TYR:CD2     | 9:J:31:GLY:N       | 2.77                     | 0.53              |
| 13:O:188:ARG:HB2   | 13:O:188:ARG:HH11  | 1.68                     | 0.53              |
| 1:a:5052:PHE:C     | 1:a:5071:LEU:HD12  | 2.33                     | 0.53              |
| 1:a:5137:LEU:HB2   | 1:a:5139:MET:HE3   | 1.89                     | 0.53              |
| 1:a:5244:GLU:CG    | 4:d:5242:GLU:HA    | 2.38                     | 0.53              |
| 1:a:5279:ARG:HE    | 23:a:6038:PHO:C2C  | 2.21                     | 0.53              |
| 25:a:6044:BCR:C8   | 25:a:6044:BCR:C33  | 2.86                     | 0.53              |
| 2:b:5068:ARG:HD3   | 22:b:6011:CLA:HED1 | 1.89                     | 0.53              |
| 2:b:5257:TRP:CE3   | 4:d:5291:LEU:HD22  | 2.43                     | 0.53              |
| 2:b:5302:TRP:C     | 2:b:5304:ALA:H     | 2.16                     | 0.53              |
| 2:b:5311:PHE:CE2   | 2:b:5317:ASN:ND2   | 2.64                     | 0.53              |
| 2:b:5383:PHE:O     | 13:o:5192:SER:HA   | 2.08                     | 0.53              |
| 22:b:6015:CLA:HAA1 | 22:b:6015:CLA:HBD  | 1.90                     | 0.53              |
| 3:c:5189:TRP:O     | 3:c:5190:ALA:C     | 2.51                     | 0.53              |
| 3:c:5450:ALA:HB1   | 3:c:5456:GLU:HB3   | 1.90                     | 0.53              |
| 3:c:5453:ALA:HB3   | 3:c:5455:PHE:CE2   | 2.42                     | 0.53              |
| 4:d:5152:VAL:HG11  | 22:d:6004:CLA:H11  | 1.90                     | 0.53              |
| 9:j:5030:TYR:CD2   | 9:j:5031:GLY:N     | 2.77                     | 0.53              |
| 13:o:5086:ARG:HG3  | 13:o:5086:ARG:NH1  | 2.22                     | 0.53              |
| 13:o:5241:PHE:HD2  | 13:o:5265:PHE:HB3  | 1.72                     | 0.53              |
| 18:y:5037:PHE:O    | 18:y:5041:VAL:HG22 | 2.08                     | 0.53              |
| 1:A:76:ASN:HD21    | 11:L:33:SER:C      | 2.15                     | 0.53              |
| 1:A:90:GLY:HA2     | 1:A:167:SER:CB     | 2.38                     | 0.53              |
| 1:A:236:GLY:O      | 1:A:237:TYR:HB2    | 2.08                     | 0.53              |
| 1:A:270:SER:HB2    | 26:A:1063:LHG:H142 | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:103:LEU:HD11   | 2:B:107:LEU:CD1    | 2.37                     | 0.53              |
| 2:B:460:LEU:O      | 4:D:280:TRP:HZ3    | 1.90                     | 0.53              |
| 22:B:1018:CLA:H8   | 22:B:1023:CLA:HBA1 | 1.91                     | 0.53              |
| 3:C:151:TRP:CE3    | 3:C:157:MET:HE1    | 2.42                     | 0.53              |
| 3:C:203:THR:H      | 3:C:235:GLY:HA3    | 1.74                     | 0.53              |
| 3:C:451:ALA:O      | 3:C:453:ALA:N      | 2.40                     | 0.53              |
| 11:L:14:ARG:O      | 11:L:18:TYR:CD2    | 2.61                     | 0.53              |
| 12:M:35:SER:O      | 12:M:36:SER:CB     | 2.56                     | 0.53              |
| 13:O:79:LYS:HE2    | 13:O:89:ALA:HB1    | 1.90                     | 0.53              |
| 13:O:146:PHE:CE2   | 13:O:261:ILE:HG21  | 2.44                     | 0.53              |
| 16:V:114:ILE:HG12  | 16:V:114:ILE:O     | 2.07                     | 0.53              |
| 1:a:5064:ARG:CZ    | 13:o:5098:THR:HG21 | 2.38                     | 0.53              |
| 1:a:5271:LEU:HG    | 1:a:5272:HIS:H     | 1.73                     | 0.53              |
| 2:b:5065:PHE:HE2   | 22:b:6012:CLA:CMA  | 1.97                     | 0.53              |
| 2:b:5248:ALA:HA    | 22:b:6011:CLA:H51  | 1.90                     | 0.53              |
| 2:b:5280:PHE:CZ    | 2:b:5312:TYR:HD1   | 2.26                     | 0.53              |
| 2:b:5394:GLN:OE1   | 15:u:5017:LEU:HD21 | 2.08                     | 0.53              |
| 2:b:5452:THR:HB    | 4:d:5291:LEU:HD13  | 1.89                     | 0.53              |
| 22:b:6013:CLA:HBC3 | 22:b:6013:CLA:CMC  | 2.38                     | 0.53              |
| 3:c:5029:GLU:HA    | 3:c:5041:ARG:HH11  | 1.74                     | 0.53              |
| 3:c:5176:VAL:O     | 3:c:5180:MET:HG3   | 2.08                     | 0.53              |
| 3:c:5216:SER:O     | 3:c:5221:GLU:O     | 2.27                     | 0.53              |
| 4:d:5019:ASP:O     | 4:d:5020:ASP:C     | 2.51                     | 0.53              |
| 4:d:5272:LEU:O     | 4:d:5276:VAL:HG22  | 2.08                     | 0.53              |
| 24:d:6042:PQ9:C24  | 24:d:6042:PQ9:H292 | 2.37                     | 0.53              |
| 13:o:5100:GLU:C    | 13:o:5102:THR:H    | 2.16                     | 0.53              |
| 15:u:5031:ASN:HD22 | 15:u:5031:ASN:C    | 2.14                     | 0.53              |
| 16:v:5038:LEU:CA   | 16:v:5095:ILE:HG22 | 2.28                     | 0.53              |
| 1:A:258:LEU:HA     | 4:D:128:ARG:HH21   | 1.72                     | 0.53              |
| 2:B:95:GLY:O       | 2:B:99:ALA:N       | 2.41                     | 0.53              |
| 2:B:283:GLU:CG     | 2:B:286:ARG:HH12   | 2.21                     | 0.53              |
| 2:B:461:LEU:O      | 2:B:464:PHE:N      | 2.37                     | 0.53              |
| 22:B:1019:CLA:CBA  | 22:B:1019:CLA:HBD  | 2.38                     | 0.53              |
| 3:C:119:LEU:HD11   | 25:C:1052:BCR:H343 | 1.89                     | 0.53              |
| 3:C:146:PHE:C      | 3:C:147:PHE:CG     | 2.85                     | 0.53              |
| 3:C:165:LEU:HD22   | 22:C:1030:CLA:HMC2 | 1.90                     | 0.53              |
| 3:C:189:TRP:O      | 3:C:190:ALA:C      | 2.51                     | 0.53              |
| 3:C:216:SER:O      | 3:C:221:GLU:O      | 2.27                     | 0.53              |
| 3:C:465:PRO:CG     | 8:I:32:PRO:HB3     | 2.38                     | 0.53              |
| 4:D:18:LEU:HD23    | 4:D:32:TRP:CH2     | 2.44                     | 0.53              |
| 4:D:29:PHE:CE2     | 4:D:31:GLY:CA      | 2.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:78:VAL:HG13    | 4:D:78:VAL:O       | 2.09                     | 0.53              |
| 5:E:77:GLU:O       | 5:E:79:PHE:N       | 2.41                     | 0.53              |
| 6:F:40:MET:CB      | 6:F:43:ILE:HD11    | 2.38                     | 0.53              |
| 7:H:12:ARG:HH11    | 7:H:12:ARG:HA      | 1.74                     | 0.53              |
| 8:I:10:ILE:H       | 8:I:10:ILE:CD1     | 2.20                     | 0.53              |
| 1:a:5051:ALA:HA    | 1:a:5055:ALA:HB2   | 1.91                     | 0.53              |
| 1:a:5130:GLN:CG    | 1:a:5144:CYS:HA    | 2.38                     | 0.53              |
| 1:a:5236:GLY:O     | 1:a:5237:TYR:HB2   | 2.08                     | 0.53              |
| 1:a:5307:ILE:HG22  | 1:a:5308:ASP:N     | 2.23                     | 0.53              |
| 1:a:5315:ASN:O     | 4:d:5063:LEU:CD2   | 2.56                     | 0.53              |
| 2:b:5019:LEU:HG    | 2:b:5023:HIS:CE1   | 2.43                     | 0.53              |
| 2:b:5400:SER:CB    | 2:b:5410:THR:HG22  | 2.37                     | 0.53              |
| 2:b:5468:TRP:HE3   | 4:d:5144:ILE:HD13  | 1.73                     | 0.53              |
| 22:c:6026:CLA:H93  | 22:c:6026:CLA:H121 | 1.90                     | 0.53              |
| 22:c:6029:CLA:HMA2 | 22:c:6029:CLA:CBA  | 2.25                     | 0.53              |
| 29:c:6057:DGD:CGA  | 28:d:6059:MGE:H232 | 2.39                     | 0.53              |
| 4:d:5302:GLU:OE1   | 13:o:5186:LYS:CD   | 2.57                     | 0.53              |
| 5:e:5077:GLU:O     | 5:e:5079:PHE:N     | 2.41                     | 0.53              |
| 8:i:5030:ARG:HG3   | 8:i:5030:ARG:HH11  | 1.72                     | 0.53              |
| 10:k:5037:PHE:HB3  | 25:k:6051:BCR:H401 | 1.89                     | 0.53              |
| 1:A:148:SER:O      | 1:A:149:ALA:C      | 2.50                     | 0.53              |
| 1:A:244:GLU:CG     | 4:D:242:GLU:HA     | 2.38                     | 0.53              |
| 1:A:316:THR:C      | 1:A:318:ALA:H      | 2.15                     | 0.53              |
| 2:B:103:LEU:HG     | 2:B:104:SER:N      | 2.24                     | 0.53              |
| 2:B:280:PHE:CZ     | 2:B:312:TYR:HD1    | 2.26                     | 0.53              |
| 2:B:453:PHE:O      | 2:B:456:ALA:HB3    | 2.08                     | 0.53              |
| 22:B:1013:CLA:HMB1 | 22:B:1014:CLA:C1   | 2.38                     | 0.53              |
| 22:B:1014:CLA:H93  | 25:B:1048:BCR:H342 | 1.89                     | 0.53              |
| 22:B:1018:CLA:H71  | 22:B:1018:CLA:H2   | 1.89                     | 0.53              |
| 3:C:56:HIS:O       | 3:C:60:ILE:HG23    | 2.08                     | 0.53              |
| 3:C:56:HIS:CE1     | 22:C:1033:CLA:HHB  | 2.44                     | 0.53              |
| 3:C:265:ILE:CG2    | 3:C:270:ALA:HB1    | 2.39                     | 0.53              |
| 22:C:1026:CLA:C12  | 22:C:1026:CLA:H93  | 2.38                     | 0.53              |
| 6:F:22:ALA:C       | 6:F:24:HIS:N       | 2.62                     | 0.53              |
| 15:U:44:THR:O      | 15:U:45:LEU:C      | 2.51                     | 0.53              |
| 16:V:119:PRO:CB    | 16:V:130:MET:HE2   | 2.39                     | 0.53              |
| 1:a:5116:ILE:CG2   | 1:a:5117:PHE:H     | 2.19                     | 0.53              |
| 1:a:5321:ILE:CD1   | 4:d:5176:ALA:HB1   | 2.17                     | 0.53              |
| 2:b:5021:ALA:HA    | 2:b:5024:LEU:HB3   | 1.89                     | 0.53              |
| 3:c:5059:LEU:CD2   | 22:k:6034:CLA:HBD  | 2.38                     | 0.53              |
| 3:c:5188:THR:HA    | 3:c:5194:GLY:HA2   | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5223:TRP:HE1   | 3:c:5224:ILE:CG1   | 2.22                     | 0.53              |
| 3:c:5466:VAL:C     | 3:c:5468:SER:H     | 2.16                     | 0.53              |
| 22:c:6031:CLA:H142 | 25:c:6054:BCR:C36  | 2.37                     | 0.53              |
| 4:d:5021:TRP:HZ3   | 17:x:5037:LEU:HD21 | 1.73                     | 0.53              |
| 4:d:5214:HIS:HA    | 4:d:5217:THR:CG2   | 2.39                     | 0.53              |
| 10:k:5034:ALA:O    | 10:k:5035:LEU:C    | 2.51                     | 0.53              |
| 13:o:5125:ASP:CG   | 13:o:5126:GLY:N    | 2.66                     | 0.53              |
| 18:y:5042:ARG:HB2  | 18:y:5043:ARG:HH11 | 1.70                     | 0.53              |
| 1:A:140:ARG:NH2    | 26:A:1063:LHG:O4   | 2.41                     | 0.53              |
| 1:A:172:MET:SD     | 1:A:179:THR:HG22   | 2.47                     | 0.53              |
| 1:A:258:LEU:HA     | 4:D:132:ILE:HD12   | 1.90                     | 0.53              |
| 3:C:59:LEU:CD2     | 22:K:1034:CLA:HBD  | 2.38                     | 0.53              |
| 3:C:65:GLY:CA      | 3:C:119:LEU:HB2    | 2.39                     | 0.53              |
| 6:F:34:LEU:HD12    | 9:J:24:ILE:HD13    | 1.90                     | 0.53              |
| 7:H:40:VAL:O       | 7:H:44:ILE:HB      | 2.08                     | 0.53              |
| 10:K:19:ASP:N      | 10:K:20:PRO:CD     | 2.72                     | 0.53              |
| 16:V:159:GLY:HA2   | 16:V:163:TYR:HE1   | 1.72                     | 0.53              |
| 18:Y:37:PHE:O      | 18:Y:41:VAL:HG22   | 2.08                     | 0.53              |
| 18:Y:39:LEU:HD22   | 20:Z:28:ALA:HB1    | 1.91                     | 0.53              |
| 20:Z:1:MET:SD      | 20:Z:4:LEU:HD23    | 2.48                     | 0.53              |
| 1:a:5138:GLY:HA2   | 3:c:5455:PHE:CE2   | 2.43                     | 0.53              |
| 2:b:5103:LEU:HG    | 2:b:5104:SER:N     | 2.23                     | 0.53              |
| 2:b:5203:ILE:HG23  | 2:b:5204:ALA:N     | 2.24                     | 0.53              |
| 2:b:5486:LEU:HD11  | 4:d:5239:GLN:HE22  | 1.74                     | 0.53              |
| 22:b:6012:CLA:HBC3 | 22:b:6012:CLA:CHD  | 2.34                     | 0.53              |
| 3:c:5322:GLN:HE22  | 3:c:5381:LYS:HA    | 1.73                     | 0.53              |
| 4:d:5078:VAL:HG13  | 4:d:5078:VAL:O     | 2.09                     | 0.53              |
| 4:d:5251:ARG:HB3   | 4:d:5251:ARG:HH11  | 1.73                     | 0.53              |
| 4:d:5284:ILE:O     | 4:d:5287:VAL:HB    | 2.09                     | 0.53              |
| 4:d:5308:ASP:C     | 4:d:5310:GLU:H     | 2.17                     | 0.53              |
| 28:d:6059:MGE:H2B1 | 28:d:6059:MGE:O1G  | 2.09                     | 0.53              |
| 6:f:5019:ARG:HH22  | 31:f:6040:HEM:CAC  | 2.17                     | 0.53              |
| 7:h:5030:LEU:HD12  | 7:h:5033:VAL:CG2   | 2.35                     | 0.53              |
| 10:k:5021:LEU:CD2  | 18:y:5024:MET:HG2  | 2.39                     | 0.53              |
| 14:t:5018:PHE:CA   | 25:t:1046:BCR:C33  | 2.82                     | 0.53              |
| 18:y:5043:ARG:NH2  | 18:y:5044:GLY:CA   | 2.72                     | 0.53              |
| 1:A:201:GLY:C      | 1:A:203:ALA:N      | 2.65                     | 0.53              |
| 2:B:25:MET:HG3     | 25:B:1045:BCR:C39  | 2.38                     | 0.53              |
| 2:B:158:LEU:HB2    | 2:B:199:VAL:HG13   | 1.90                     | 0.53              |
| 22:B:1022:CLA:C1   | 22:B:1022:CLA:H203 | 2.38                     | 0.53              |
| 22:C:1025:CLA:CED  | 22:C:1025:CLA:CAD  | 2.86                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1026:CLA:H93  | 22:C:1026:CLA:H121 | 1.90                     | 0.53              |
| 4:D:209:LEU:HD23   | 4:D:209:LEU:C      | 2.33                     | 0.53              |
| 5:E:10:PHE:CZ      | 6:F:19:ARG:HD2     | 2.43                     | 0.53              |
| 6:F:24:HIS:O       | 6:F:28:VAL:HG23    | 2.09                     | 0.53              |
| 31:F:1040:HEM:CMA  | 31:F:1040:HEM:CBA  | 2.60                     | 0.53              |
| 16:V:148:GLU:CA    | 16:V:151:ILE:HD11  | 2.29                     | 0.53              |
| 16:V:149:PRO:HB3   | 16:V:156:TRP:CD1   | 2.44                     | 0.53              |
| 1:a:5076:ASN:CB    | 1:a:5079:THR:HG23  | 2.39                     | 0.53              |
| 22:b:6012:CLA:HMD2 | 22:b:6020:CLA:C20  | 2.37                     | 0.53              |
| 28:b:6060:MGE:H5A2 | 28:b:6060:MGE:H261 | 1.91                     | 0.53              |
| 3:c:5050:LEU:HD23  | 3:c:5051:GLY:CA    | 2.39                     | 0.53              |
| 3:c:5072:LEU:HD22  | 10:k:5011:LEU:HD23 | 1.91                     | 0.53              |
| 3:c:5194:GLY:O     | 3:c:5195:ASP:HB2   | 2.09                     | 0.53              |
| 3:c:5451:ALA:N     | 3:c:5456:GLU:HG2   | 2.22                     | 0.53              |
| 4:d:5029:PHE:CE2   | 4:d:5031:GLY:CA    | 2.91                     | 0.53              |
| 4:d:5043:LEU:HD13  | 25:d:6050:BCR:H322 | 1.91                     | 0.53              |
| 4:d:5161:PRO:HB3   | 4:d:5170:ALA:HB2   | 1.90                     | 0.53              |
| 4:d:5210:LEU:HD22  | 4:d:5274:VAL:HG21  | 1.90                     | 0.53              |
| 5:e:5010:PHE:CZ    | 6:f:5019:ARG:HD2   | 2.43                     | 0.53              |
| 7:h:5038:PHE:HB2   | 25:h:6049:BCR:C10  | 2.34                     | 0.53              |
| 16:v:5068:VAL:HG13 | 16:v:5073:LYS:HE3  | 1.90                     | 0.53              |
| 1:A:130:GLN:CG     | 1:A:144:CYS:HA     | 2.38                     | 0.53              |
| 2:B:75:TRP:CD1     | 2:B:75:TRP:H       | 2.27                     | 0.53              |
| 2:B:196:GLY:C      | 2:B:198:VAL:H      | 2.17                     | 0.53              |
| 2:B:306:PRO:HG2    | 2:B:309:LEU:HB3    | 1.90                     | 0.53              |
| 2:B:452:THR:HB     | 4:D:291:LEU:HD13   | 1.89                     | 0.53              |
| 22:B:1010:CLA:O2D  | 22:B:1010:CLA:CGA  | 2.57                     | 0.53              |
| 22:B:1011:CLA:C9   | 22:B:1011:CLA:CBB  | 2.86                     | 0.53              |
| 3:C:84:GLN:O       | 3:C:86:LEU:N       | 2.41                     | 0.53              |
| 3:C:160:ILE:HG22   | 22:C:1031:CLA:HMD1 | 1.89                     | 0.53              |
| 3:C:171:GLY:O      | 3:C:172:ALA:C      | 2.52                     | 0.53              |
| 3:C:290:VAL:HG21   | 3:C:426:LEU:HD23   | 1.91                     | 0.53              |
| 4:D:58:TRP:NE1     | 5:E:64:PRO:HD2     | 2.21                     | 0.53              |
| 4:D:209:LEU:O      | 4:D:213:ILE:HG22   | 2.09                     | 0.53              |
| 28:D:1059:MGE:O1G  | 28:D:1059:MGE:H2B1 | 2.09                     | 0.53              |
| 11:L:15:THR:HG22   | 11:L:16:SER:N      | 2.23                     | 0.53              |
| 25:T:6048:BCR:H403 | 25:T:6048:BCR:C22  | 2.34                     | 0.53              |
| 1:a:5045:THR:CG2   | 1:a:5046:ILE:N     | 2.71                     | 0.53              |
| 1:a:5130:GLN:HG2   | 1:a:5144:CYS:HA    | 1.89                     | 0.53              |
| 1:a:5269:ARG:CD    | 4:d:5222:LEU:HD11  | 2.28                     | 0.53              |
| 24:a:6043:PQ9:H293 | 23:d:6039:PHO:HBA1 | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5118:GLY:O     | 4:d:5122:LEU:HD22  | 2.08                     | 0.53              |
| 12:m:5035:SER:O    | 12:m:5036:SER:CB   | 2.56                     | 0.53              |
| 16:v:5040:SER:HB3  | 16:v:5094:ASN:HD21 | 1.74                     | 0.53              |
| 16:v:5106:THR:CA   | 16:v:5114:ILE:HG22 | 2.38                     | 0.53              |
| 16:v:5149:PRO:HB3  | 16:v:5156:TRP:CD1  | 2.44                     | 0.53              |
| 1:A:47:CYS:SG      | 1:A:115:ILE:HD11   | 2.49                     | 0.53              |
| 1:A:52:PHE:C       | 1:A:71:LEU:HD12    | 2.33                     | 0.53              |
| 1:A:305:SER:HB3    | 3:C:415:ASN:ND2    | 2.24                     | 0.53              |
| 22:A:1007:CLA:HAC1 | 25:A:1044:BCR:C15  | 2.38                     | 0.53              |
| 24:A:1043:PQ9:H453 | 24:A:1043:PQ9:C40  | 2.39                     | 0.53              |
| 2:B:246:PHE:CD1    | 2:B:247:PHE:N      | 2.77                     | 0.53              |
| 2:B:278:SER:HB3    | 2:B:281:GLN:CG     | 2.28                     | 0.53              |
| 2:B:425:ILE:HG23   | 2:B:425:ILE:O      | 2.09                     | 0.53              |
| 2:B:460:LEU:HG     | 29:B:1058:DGD:HAG3 | 1.91                     | 0.53              |
| 22:B:1013:CLA:HBC3 | 22:B:1013:CLA:CMC  | 2.38                     | 0.53              |
| 3:C:117:VAL:CG1    | 22:C:1027:CLA:H42  | 2.32                     | 0.53              |
| 3:C:340:TYR:CD2    | 3:C:340:TYR:N      | 2.70                     | 0.53              |
| 22:C:1031:CLA:HMA2 | 22:C:1031:CLA:C1   | 2.38                     | 0.53              |
| 4:D:19:ASP:O       | 4:D:20:ASP:C       | 2.51                     | 0.53              |
| 4:D:21:TRP:HZ3     | 17:X:37:LEU:HD21   | 1.73                     | 0.53              |
| 4:D:249:ALA:HB1    | 24:D:1042:PQ9:C6   | 2.39                     | 0.53              |
| 10:K:38:VAL:HG12   | 10:K:39:VAL:N      | 2.23                     | 0.53              |
| 11:L:23:LEU:O      | 11:L:27:LEU:HG     | 2.09                     | 0.53              |
| 16:V:39:ASN:ND2    | 16:V:40:SER:N      | 2.54                     | 0.53              |
| 1:a:5058:VAL:HG21  | 1:a:5083:VAL:HG23  | 1.91                     | 0.53              |
| 1:a:5225:ARG:HB2   | 2:b:5484:PRO:HD3   | 1.91                     | 0.53              |
| 1:a:5279:ARG:O     | 1:a:5283:VAL:HG23  | 2.09                     | 0.53              |
| 26:a:6063:LHG:H242 | 22:c:6032:CLA:OBD  | 2.09                     | 0.53              |
| 2:b:5061:PHE:C     | 2:b:5064:PRO:HD2   | 2.34                     | 0.53              |
| 2:b:5075:TRP:CD1   | 2:b:5075:TRP:H     | 2.27                     | 0.53              |
| 22:b:6009:CLA:CGA  | 22:b:6009:CLA:CHA  | 2.87                     | 0.53              |
| 3:c:5065:GLY:CA    | 3:c:5119:LEU:HB2   | 2.39                     | 0.53              |
| 3:c:5185:LEU:HG    | 3:c:5199:ILE:CD1   | 2.37                     | 0.53              |
| 3:c:5203:THR:H     | 3:c:5235:GLY:HA3   | 1.74                     | 0.53              |
| 6:f:5024:HIS:O     | 6:f:5028:VAL:HG23  | 2.09                     | 0.53              |
| 7:h:5030:LEU:HA    | 7:h:5033:VAL:HG22  | 1.91                     | 0.53              |
| 7:h:5040:VAL:O     | 7:h:5044:ILE:HB    | 2.08                     | 0.53              |
| 16:v:5118:HIS:CD2  | 16:v:5119:PRO:CD   | 2.85                     | 0.53              |
| 16:v:5138:LEU:O    | 16:v:5139:VAL:C    | 2.50                     | 0.53              |
| 16:v:5148:GLU:CA   | 16:v:5151:ILE:HD11 | 2.29                     | 0.53              |
| 1:A:216:GLY:O      | 4:D:268:HIS:O      | 2.27                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:A:1043:PQ9:H293 | 23:D:1039:PHO:HBA1 | 1.91                     | 0.53              |
| 2:B:26:HIS:NE2     | 22:B:1021:CLA:NB   | 2.57                     | 0.53              |
| 2:B:61:PHE:C       | 2:B:64:PRO:HD2     | 2.34                     | 0.53              |
| 22:B:1019:CLA:HMA2 | 22:B:1020:CLA:CMC  | 2.39                     | 0.53              |
| 3:C:188:THR:HA     | 3:C:194:GLY:HA2    | 1.90                     | 0.53              |
| 4:D:152:VAL:HG11   | 22:D:1004:CLA:H11  | 1.90                     | 0.53              |
| 4:D:272:LEU:O      | 4:D:276:VAL:HG22   | 2.08                     | 0.53              |
| 23:D:1039:PHO:C4   | 23:D:1039:PHO:CGA  | 2.87                     | 0.53              |
| 7:H:31:MET:HB2     | 22:H:1017:CLA:C3D  | 2.38                     | 0.53              |
| 13:O:214:LYS:HE3   | 13:O:251:MET:CG    | 2.34                     | 0.53              |
| 18:Y:35:ILE:HD13   | 18:Y:35:ILE:C      | 2.34                     | 0.53              |
| 18:Y:35:ILE:HD13   | 18:Y:36:ILE:N      | 2.24                     | 0.53              |
| 18:Y:43:ARG:NH2    | 18:Y:44:GLY:CA     | 2.72                     | 0.53              |
| 1:a:5134:SER:OG    | 1:a:5141:PRO:HB3   | 2.09                     | 0.53              |
| 1:a:5285:PHE:HA    | 1:a:5288:LEU:HD12  | 1.90                     | 0.53              |
| 1:a:5335:ASN:ND2   | 13:o:5182:PHE:CD1  | 2.77                     | 0.53              |
| 2:b:5134:ASP:O     | 2:b:5138:MET:HB2   | 2.09                     | 0.53              |
| 2:b:5460:LEU:HG    | 29:b:6058:DGD:HAG3 | 1.91                     | 0.53              |
| 22:b:6020:CLA:C1   | 22:b:6023:CLA:O1A  | 2.55                     | 0.53              |
| 4:d:5067:TYR:CE1   | 28:d:6059:MGE:H1G1 | 2.44                     | 0.53              |
| 4:d:5209:LEU:O     | 4:d:5213:ILE:HG22  | 2.09                     | 0.53              |
| 4:d:5213:ILE:HG23  | 4:d:5214:HIS:N     | 2.23                     | 0.53              |
| 4:d:5275:PRO:O     | 4:d:5276:VAL:C     | 2.52                     | 0.53              |
| 6:f:5022:ALA:C     | 6:f:5024:HIS:H     | 2.17                     | 0.53              |
| 13:o:5224:SER:C    | 13:o:5225:LEU:HD12 | 2.33                     | 0.53              |
| 25:t:1046:BCR:H23C | 25:t:1046:BCR:C39  | 2.26                     | 0.53              |
| 1:A:51:ALA:HA      | 1:A:55:ALA:HB2     | 1.91                     | 0.53              |
| 1:A:146:ALA:HA     | 1:A:280:VAL:HG11   | 1.91                     | 0.53              |
| 1:A:225:ARG:HB2    | 2:B:484:PRO:HD3    | 1.91                     | 0.53              |
| 26:A:1063:LHG:H242 | 22:C:1032:CLA:OBD  | 2.09                     | 0.53              |
| 2:B:30:VAL:O       | 2:B:31:ALA:C       | 2.50                     | 0.53              |
| 2:B:62:VAL:HG13    | 22:B:1013:CLA:O1D  | 2.09                     | 0.53              |
| 2:B:79:SER:OG      | 2:B:80:ILE:N       | 2.41                     | 0.53              |
| 3:C:50:LEU:HD23    | 3:C:51:GLY:CA      | 2.39                     | 0.53              |
| 3:C:88:LEU:C       | 3:C:90:PRO:HD2     | 2.34                     | 0.53              |
| 4:D:36:LEU:HD21    | 4:D:124:GLY:HA3    | 1.91                     | 0.53              |
| 4:D:43:LEU:HD13    | 25:D:1050:BCR:H322 | 1.91                     | 0.53              |
| 4:D:182:LEU:N      | 4:D:182:LEU:HD23   | 2.24                     | 0.53              |
| 24:D:1042:PQ9:C23  | 28:L:1061:MGE:CGB  | 2.87                     | 0.53              |
| 5:E:43:ALA:O       | 5:E:46:VAL:HB      | 2.08                     | 0.53              |
| 11:L:32:SER:OG     | 11:L:33:SER:N      | 2.42                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:M:9:ILE:HG23    | 12:M:13:LEU:CD2    | 2.39                     | 0.53              |
| 13:O:63:THR:CG2    | 13:O:271:PRO:O     | 2.57                     | 0.53              |
| 1:a:5180:PHE:CE1   | 4:d:5192:THR:O     | 2.61                     | 0.53              |
| 2:b:5025:MET:CG    | 25:b:6045:BCR:H401 | 2.35                     | 0.53              |
| 2:b:5196:GLY:C     | 2:b:5198:VAL:H     | 2.17                     | 0.53              |
| 2:b:5220:ARG:HD3   | 2:b:5221:PRO:CD    | 2.29                     | 0.53              |
| 22:b:6011:CLA:CGA  | 22:b:6011:CLA:C4   | 2.87                     | 0.53              |
| 22:b:6013:CLA:HMB1 | 22:b:6014:CLA:C1   | 2.39                     | 0.53              |
| 4:d:5172:SER:O     | 4:d:5173:PHE:HB2   | 2.08                     | 0.53              |
| 4:d:5274:VAL:HG12  | 4:d:5275:PRO:N     | 2.24                     | 0.53              |
| 22:d:6005:CLA:CBA  | 24:d:6042:PQ9:H412 | 2.38                     | 0.53              |
| 24:d:6042:PQ9:C23  | 28:l:6061:MGE:CGB  | 2.87                     | 0.53              |
| 15:u:5021:TYR:HE2  | 15:u:5030:THR:HG1  | 1.55                     | 0.53              |
| 1:A:17:PHE:CZ      | 8:I:18:LEU:HD11    | 2.44                     | 0.52              |
| 1:A:40:THR:H       | 22:A:1007:CLA:HBB1 | 1.75                     | 0.52              |
| 1:A:134:SER:OG     | 1:A:141:PRO:HB3    | 2.09                     | 0.52              |
| 1:A:199:GLN:C      | 1:A:201:GLY:N      | 2.67                     | 0.52              |
| 1:A:279:ARG:O      | 1:A:283:VAL:HG23   | 2.09                     | 0.52              |
| 22:A:1007:CLA:H43  | 22:C:1029:CLA:H192 | 1.89                     | 0.52              |
| 22:A:1007:CLA:H142 | 8:I:13:THR:HG21    | 1.91                     | 0.52              |
| 2:B:45:PHE:HA      | 2:B:58:GLN:NE2     | 2.23                     | 0.52              |
| 22:B:1012:CLA:CHD  | 22:B:1020:CLA:H201 | 2.37                     | 0.52              |
| 22:B:1022:CLA:H43  | 22:B:1022:CLA:O2A  | 2.10                     | 0.52              |
| 3:C:405:ASN:OD1    | 29:C:1057:DGD:HD61 | 2.09                     | 0.52              |
| 3:C:417:VAL:HG11   | 16:V:68:VAL:HG12   | 1.86                     | 0.52              |
| 22:C:1032:CLA:H62  | 22:C:1032:CLA:H112 | 1.91                     | 0.52              |
| 4:D:67:TYR:CE1     | 28:D:1059:MGE:H1G1 | 2.44                     | 0.52              |
| 4:D:302:GLU:OE1    | 13:O:186:LYS:CD    | 2.57                     | 0.52              |
| 6:F:22:ALA:C       | 6:F:24:HIS:H       | 2.17                     | 0.52              |
| 13:O:224:SER:C     | 13:O:225:LEU:HD12  | 2.33                     | 0.52              |
| 25:T:6046:BCR:H23C | 25:T:6046:BCR:C39  | 2.26                     | 0.52              |
| 20:Z:5:PHE:CE1     | 20:Z:54:VAL:HG13   | 2.42                     | 0.52              |
| 1:a:5058:VAL:HB    | 1:a:5083:VAL:HG21  | 1.90                     | 0.52              |
| 1:a:5140:ARG:NH2   | 26:a:6063:LHG:O4   | 2.41                     | 0.52              |
| 1:a:5179:THR:O     | 1:a:5180:PHE:C     | 2.52                     | 0.52              |
| 1:a:5218:LEU:HD11  | 1:a:5255:PHE:HB2   | 1.90                     | 0.52              |
| 2:b:5246:PHE:CD1   | 2:b:5247:PHE:N     | 2.77                     | 0.52              |
| 22:b:6010:CLA:O2D  | 22:b:6010:CLA:CGA  | 2.57                     | 0.52              |
| 22:b:6016:CLA:H193 | 22:h:6017:CLA:C19  | 2.15                     | 0.52              |
| 22:b:6022:CLA:H43  | 22:b:6022:CLA:O2A  | 2.09                     | 0.52              |
| 3:c:5049:LEU:HD11  | 22:c:6035:CLA:HMA3 | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5084:GLN:O     | 3:c:5086:LEU:N     | 2.42                     | 0.52              |
| 3:c:5137:PRO:C     | 3:c:5139:THR:N     | 2.66                     | 0.52              |
| 3:c:5155:ASN:HA    | 3:c:5158:THR:CG2   | 2.29                     | 0.52              |
| 4:d:5018:LEU:HD23  | 4:d:5032:TRP:CH2   | 2.44                     | 0.52              |
| 4:d:5088:SER:C     | 4:d:5090:LEU:H     | 2.17                     | 0.52              |
| 5:e:5010:PHE:O     | 5:e:5011:SER:C     | 2.51                     | 0.52              |
| 12:m:5009:ILE:HG23 | 12:m:5013:LEU:CD2  | 2.39                     | 0.52              |
| 18:y:5035:ILE:C    | 18:y:5035:ILE:HD13 | 2.34                     | 0.52              |
| 18:y:5035:ILE:HD13 | 18:y:5036:ILE:N    | 2.24                     | 0.52              |
| 1:A:223:LEU:CD2    | 4:D:265:ARG:HG2    | 2.35                     | 0.52              |
| 1:A:224:ILE:HA     | 2:B:482:ILE:HG13   | 1.91                     | 0.52              |
| 1:A:285:PHE:HA     | 1:A:288:LEU:HD12   | 1.90                     | 0.52              |
| 1:A:297:LEU:HD12   | 3:C:428:THR:HG21   | 1.91                     | 0.52              |
| 1:A:316:THR:HG22   | 4:D:75:THR:HG23    | 1.91                     | 0.52              |
| 26:A:1063:LHG:H292 | 22:C:1032:CLA:C5   | 2.27                     | 0.52              |
| 2:B:49:ASP:HB3     | 13:o:5083:LYS:HE3  | 1.89                     | 0.52              |
| 2:B:106:LEU:HD12   | 25:B:1048:BCR:H352 | 1.91                     | 0.52              |
| 2:B:275:TRP:HB3    | 2:B:318:ASN:HD22   | 1.75                     | 0.52              |
| 22:B:1009:CLA:CGA  | 22:B:1009:CLA:CHA  | 2.87                     | 0.52              |
| 25:B:1047:BCR:C30  | 25:B:1047:BCR:C37  | 2.61                     | 0.52              |
| 4:D:32:TRP:HE3     | 4:D:35:ILE:HD11    | 1.72                     | 0.52              |
| 4:D:189:HIS:O      | 4:D:190:ASN:C      | 2.52                     | 0.52              |
| 4:D:210:LEU:HD22   | 4:D:274:VAL:HG21   | 1.90                     | 0.52              |
| 5:E:13:ILE:CD1     | 5:E:19:TYR:HB2     | 2.40                     | 0.52              |
| 5:E:17:VAL:HG13    | 9:J:8:ILE:HD11     | 1.91                     | 0.52              |
| 7:H:35:MET:HA      | 25:H:1049:BCR:C33  | 2.39                     | 0.52              |
| 25:H:1049:BCR:HC8  | 25:H:1049:BCR:C31  | 2.26                     | 0.52              |
| 9:J:20:GLY:O       | 9:J:23:VAL:HG12    | 2.09                     | 0.52              |
| 16:V:40:SER:HB3    | 16:V:94:ASN:HD21   | 1.74                     | 0.52              |
| 18:Y:35:ILE:HD13   | 18:Y:36:ILE:HD12   | 1.91                     | 0.52              |
| 1:a:5091:LEU:O     | 1:a:5092:HIS:C     | 2.50                     | 0.52              |
| 1:a:5107:TYR:CD2   | 13:o:5097:VAL:HG11 | 2.44                     | 0.52              |
| 1:a:5328:MET:CE    | 4:d:5183:LEU:HD13  | 2.39                     | 0.52              |
| 25:a:6044:BCR:H331 | 25:a:6044:BCR:C34  | 2.39                     | 0.52              |
| 22:b:6018:CLA:C10  | 22:b:6023:CLA:CBA  | 2.85                     | 0.52              |
| 22:b:6019:CLA:CBA  | 22:b:6019:CLA:HBD  | 2.38                     | 0.52              |
| 3:c:5050:LEU:CD2   | 3:c:5051:GLY:CA    | 2.87                     | 0.52              |
| 3:c:5056:HIS:O     | 3:c:5060:ILE:HG23  | 2.08                     | 0.52              |
| 4:d:5259:ILE:HG22  | 4:d:5260:ALA:N     | 2.23                     | 0.52              |
| 5:e:5047:PHE:O     | 5:e:5049:THR:N     | 2.41                     | 0.52              |
| 7:h:5012:ARG:HA    | 7:h:5012:ARG:HH11  | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:u:5042:TYR:O    | 15:u:5043:PRO:C    | 2.50                     | 0.52              |
| 18:y:5039:LEU:HD22 | 20:z:5028:ALA:HB1  | 1.91                     | 0.52              |
| 1:A:140:ARG:HH11   | 1:A:140:ARG:HB2    | 1.74                     | 0.52              |
| 1:A:269:ARG:CD     | 4:D:222:LEU:HD11   | 2.28                     | 0.52              |
| 1:A:283:VAL:HG21   | 23:A:1038:PHO:HMC3 | 1.90                     | 0.52              |
| 1:A:335:ASN:ND2    | 13:O:182:PHE:CD1   | 2.77                     | 0.52              |
| 2:B:486:LEU:HD11   | 4:D:239:GLN:HE22   | 1.74                     | 0.52              |
| 3:C:165:LEU:HB2    | 3:C:248:GLY:HA3    | 1.90                     | 0.52              |
| 3:C:176:VAL:O      | 3:C:180:MET:HG3    | 2.08                     | 0.52              |
| 3:C:185:LEU:HG     | 3:C:199:ILE:CD1    | 2.37                     | 0.52              |
| 3:C:314:ALA:HB1    | 3:C:351:PHE:CD1    | 2.45                     | 0.52              |
| 3:C:315:MET:O      | 3:C:319:ILE:HG13   | 2.10                     | 0.52              |
| 22:C:1033:CLA:C14  | 22:C:1036:CLA:C2D  | 2.87                     | 0.52              |
| 4:D:82:ALA:C       | 4:D:84:SER:H       | 2.16                     | 0.52              |
| 4:D:118:GLY:O      | 4:D:122:LEU:HD22   | 2.09                     | 0.52              |
| 4:D:172:SER:O      | 4:D:173:PHE:HB2    | 2.08                     | 0.52              |
| 4:D:265:ARG:O      | 4:D:265:ARG:HD3    | 2.10                     | 0.52              |
| 4:D:275:PRO:O      | 4:D:276:VAL:C      | 2.52                     | 0.52              |
| 13:O:92:VAL:HG11   | 13:O:137:ALA:HB2   | 1.90                     | 0.52              |
| 16:V:39:ASN:C      | 16:V:41:GLU:N      | 2.67                     | 0.52              |
| 1:a:5017:PHE:CZ    | 8:i:5018:LEU:HD11  | 2.44                     | 0.52              |
| 1:a:5140:ARG:HH11  | 1:a:5140:ARG:HB2   | 1.74                     | 0.52              |
| 1:a:5288:LEU:O     | 1:a:5292:THR:N     | 2.42                     | 0.52              |
| 24:a:6043:PQ9:H453 | 24:a:6043:PQ9:C40  | 2.39                     | 0.52              |
| 2:b:5475:PHE:C     | 2:b:5477:ASP:H     | 2.16                     | 0.52              |
| 3:c:5369:LEU:HD13  | 3:c:5380:ILE:CD1   | 2.37                     | 0.52              |
| 22:c:6033:CLA:C14  | 22:c:6036:CLA:C2D  | 2.87                     | 0.52              |
| 29:c:6056:DGD:HB1  | 29:c:6056:DGD:C8B  | 2.39                     | 0.52              |
| 5:e:5043:ALA:O     | 5:e:5046:VAL:HB    | 2.08                     | 0.52              |
| 14:t:5019:PHE:N    | 14:t:5019:PHE:CD2  | 2.77                     | 0.52              |
| 20:z:5053:VAL:C    | 20:z:5055:GLY:H    | 2.17                     | 0.52              |
| 1:A:37:MET:O       | 1:A:38:ILE:C       | 2.51                     | 0.52              |
| 1:A:296:ASN:HB3    | 3:C:401:LEU:HD13   | 1.91                     | 0.52              |
| 2:B:25:MET:CG      | 25:B:1045:BCR:H391 | 2.37                     | 0.52              |
| 2:B:25:MET:CG      | 25:B:1045:BCR:H401 | 2.35                     | 0.52              |
| 2:B:169:SER:CB     | 2:B:176:GLY:HA2    | 2.17                     | 0.52              |
| 3:C:50:LEU:CD2     | 3:C:51:GLY:CA      | 2.87                     | 0.52              |
| 3:C:223:TRP:NE1    | 3:C:224:ILE:CG1    | 2.69                     | 0.52              |
| 3:C:223:TRP:HE1    | 3:C:224:ILE:CG1    | 2.22                     | 0.52              |
| 22:C:1029:CLA:H11  | 22:C:1029:CLA:CHA  | 2.39                     | 0.52              |
| 22:C:1035:CLA:HMC3 | 22:K:1034:CLA:HMB3 | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:C:1057:DGD:CGA  | 28:D:1059:MGE:H232 | 2.39                     | 0.52              |
| 4:D:33:SER:O       | 4:D:34:GLY:C       | 2.52                     | 0.52              |
| 24:D:1042:PQ9:H252 | 28:L:1061:MGE:H261 | 1.92                     | 0.52              |
| 10:K:14:ALA:H      | 20:Z:62:VAL:HG11   | 1.73                     | 0.52              |
| 11:L:29:LEU:CB     | 14:T:9:ILE:HG21    | 2.32                     | 0.52              |
| 15:U:16:LYS:HG2    | 15:U:21:TYR:HD1    | 1.74                     | 0.52              |
| 16:V:144:HIS:CD2   | 16:V:148:GLU:HG3   | 2.44                     | 0.52              |
| 17:X:36:VAL:O      | 17:X:39:ALA:HB3    | 2.10                     | 0.52              |
| 20:Z:53:VAL:C      | 20:Z:55:GLY:H      | 2.17                     | 0.52              |
| 1:a:5047:CYS:SG    | 1:a:5115:ILE:HD11  | 2.49                     | 0.52              |
| 1:a:5181:ASN:HA    | 4:d:5318:ASN:OD1   | 2.09                     | 0.52              |
| 1:a:5258:LEU:HA    | 4:d:5132:ILE:HD12  | 1.90                     | 0.52              |
| 1:a:5305:SER:HB3   | 3:c:5415:ASN:ND2   | 2.24                     | 0.52              |
| 2:b:5062:VAL:HG13  | 22:b:6013:CLA:O1D  | 2.09                     | 0.52              |
| 2:b:5265:ILE:H     | 2:b:5265:ILE:CD1   | 2.05                     | 0.52              |
| 3:c:5088:LEU:C     | 3:c:5090:PRO:HD2   | 2.34                     | 0.52              |
| 3:c:5165:LEU:HB2   | 3:c:5248:GLY:HA3   | 1.90                     | 0.52              |
| 3:c:5290:VAL:HG21  | 3:c:5426:LEU:HD23  | 1.91                     | 0.52              |
| 22:c:6035:CLA:HMC3 | 22:k:6034:CLA:HMB3 | 1.91                     | 0.52              |
| 4:d:5033:SER:O     | 4:d:5034:GLY:C     | 2.52                     | 0.52              |
| 4:d:5036:LEU:HD21  | 4:d:5124:GLY:HA3   | 1.91                     | 0.52              |
| 4:d:5250:ASN:C     | 4:d:5252:PHE:H     | 2.17                     | 0.52              |
| 23:d:6039:PHO:C4   | 23:d:6039:PHO:CGA  | 2.87                     | 0.52              |
| 13:o:5082:PRO:HG2  | 13:o:5089:ALA:HB1  | 1.87                     | 0.52              |
| 25:t:1046:BCR:C23  | 25:t:1046:BCR:C39  | 2.83                     | 0.52              |
| 16:v:5119:PRO:HB2  | 16:v:5130:MET:HE2  | 1.92                     | 0.52              |
| 16:v:5144:HIS:CD2  | 16:v:5148:GLU:HG3  | 2.44                     | 0.52              |
| 25:A:1044:BCR:H331 | 25:A:1044:BCR:C34  | 2.39                     | 0.52              |
| 2:B:190:PHE:CZ     | 22:B:1009:CLA:HMA1 | 2.45                     | 0.52              |
| 2:B:235:GLU:HG3    | 2:B:473:THR:OG1    | 2.09                     | 0.52              |
| 2:B:354:LEU:CD2    | 2:B:378:LYS:HB2    | 2.40                     | 0.52              |
| 2:B:372:ASP:OD2    | 2:B:376:VAL:HG23   | 2.10                     | 0.52              |
| 2:B:463:PHE:C      | 2:B:463:PHE:CD2    | 2.87                     | 0.52              |
| 3:C:209:ILE:HD13   | 3:C:236:GLY:HA2    | 1.90                     | 0.52              |
| 22:C:1027:CLA:HBC3 | 22:C:1027:CLA:CMC  | 2.39                     | 0.52              |
| 25:C:1052:BCR:C38  | 25:C:1052:BCR:H372 | 2.23                     | 0.52              |
| 29:C:1056:DGD:HB1  | 29:C:1056:DGD:C8B  | 2.39                     | 0.52              |
| 4:D:185:PHE:CE1    | 22:D:1004:CLA:HMD2 | 2.44                     | 0.52              |
| 4:D:214:HIS:HA     | 4:D:217:THR:CG2    | 2.40                     | 0.52              |
| 4:D:284:ILE:O      | 4:D:287:VAL:HB     | 2.09                     | 0.52              |
| 7:H:30:LEU:HA      | 7:H:33:VAL:HG22    | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:K:21:LEU:CD2    | 18:Y:24:MET:HG2    | 2.39                     | 0.52              |
| 12:M:34:LYS:HE2    | 11:l:5009:PRO:HB2  | 1.91                     | 0.52              |
| 25:T:6046:BCR:H391 | 25:b:6047:BCR:H14C | 1.90                     | 0.52              |
| 15:U:50:VAL:C      | 15:U:51:LYS:O      | 2.46                     | 0.52              |
| 16:V:106:THR:CA    | 16:V:114:ILE:HG22  | 2.38                     | 0.52              |
| 16:V:108:TYR:O     | 16:V:108:TYR:HD2   | 1.93                     | 0.52              |
| 16:V:118:HIS:CD2   | 16:V:119:PRO:CD    | 2.85                     | 0.52              |
| 1:a:5246:TYR:CD1   | 1:a:5246:TYR:N     | 2.73                     | 0.52              |
| 1:a:5316:THR:HG22  | 4:d:5075:THR:HG23  | 1.91                     | 0.52              |
| 1:a:5331:MET:HA    | 1:a:5331:MET:HE3   | 1.91                     | 0.52              |
| 22:a:6003:CLA:HED2 | 22:a:6003:CLA:CBA  | 2.32                     | 0.52              |
| 2:b:5024:LEU:HD22  | 2:b:5114:HIS:HD2   | 1.75                     | 0.52              |
| 2:b:5215:PHE:C     | 2:b:5215:PHE:CD2   | 2.88                     | 0.52              |
| 22:b:6016:CLA:H51  | 22:h:6017:CLA:H91  | 1.76                     | 0.52              |
| 22:b:6020:CLA:C16  | 22:b:6020:CLA:H111 | 2.39                     | 0.52              |
| 3:c:5265:ILE:CG2   | 3:c:5270:ALA:HB1   | 2.39                     | 0.52              |
| 4:d:5186:GLN:H     | 22:d:6004:CLA:HBC1 | 1.75                     | 0.52              |
| 23:d:6039:PHO:H42  | 23:d:6039:PHO:CGA  | 2.39                     | 0.52              |
| 5:e:5059:GLU:OE1   | 5:e:5059:GLU:HA    | 2.09                     | 0.52              |
| 7:h:5038:PHE:O     | 7:h:5041:PHE:N     | 2.40                     | 0.52              |
| 10:k:5019:ASP:N    | 10:k:5020:PRO:CD   | 2.72                     | 0.52              |
| 25:k:6052:BCR:C34  | 25:k:6051:BCR:HC21 | 2.39                     | 0.52              |
| 16:v:5045:ILE:H    | 16:v:5045:ILE:CD1  | 2.06                     | 0.52              |
| 18:y:5035:ILE:HD13 | 18:y:5036:ILE:HD12 | 1.91                     | 0.52              |
| 1:A:76:ASN:CB      | 1:A:79:THR:HG23    | 2.39                     | 0.52              |
| 1:A:181:ASN:HA     | 4:D:318:ASN:OD1    | 2.09                     | 0.52              |
| 1:A:328:MET:CE     | 4:D:183:LEU:HD13   | 2.39                     | 0.52              |
| 2:B:15:ASP:OD2     | 2:B:18:ARG:HG3     | 2.09                     | 0.52              |
| 2:B:134:ASP:O      | 2:B:138:MET:HB2    | 2.09                     | 0.52              |
| 2:B:302:TRP:C      | 2:B:304:ALA:H      | 2.16                     | 0.52              |
| 2:B:483:ASP:O      | 2:B:485:GLU:N      | 2.43                     | 0.52              |
| 22:B:1011:CLA:CGA  | 22:B:1011:CLA:C4   | 2.87                     | 0.52              |
| 25:B:1045:BCR:C38  | 25:B:1045:BCR:C23  | 2.71                     | 0.52              |
| 3:C:466:VAL:C      | 3:C:468:SER:H      | 2.16                     | 0.52              |
| 22:D:1005:CLA:O1A  | 22:D:1005:CLA:NA   | 2.43                     | 0.52              |
| 23:D:1039:PHO:H42  | 23:D:1039:PHO:CGA  | 2.39                     | 0.52              |
| 6:F:38:ALA:HA      | 9:J:27:LEU:HD21    | 1.91                     | 0.52              |
| 13:O:250:ASP:O     | 13:O:252:GLY:N     | 2.35                     | 0.52              |
| 15:U:16:LYS:NZ     | 15:U:85:THR:HB     | 2.25                     | 0.52              |
| 1:a:5017:PHE:O     | 1:a:5021:VAL:HG23  | 2.10                     | 0.52              |
| 1:a:5040:THR:H     | 22:a:6007:CLA:HBB1 | 1.75                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5180:PHE:CZ    | 4:d:5192:THR:O     | 2.63                     | 0.52              |
| 2:b:5030:VAL:CG1   | 22:b:6013:CLA:HHD  | 2.40                     | 0.52              |
| 2:b:5067:ALA:HB3   | 2:b:5267:LEU:CD1   | 2.40                     | 0.52              |
| 2:b:5235:GLU:HG3   | 2:b:5473:THR:OG1   | 2.09                     | 0.52              |
| 22:b:6021:CLA:HED3 | 22:b:6021:CLA:HMA3 | 1.91                     | 0.52              |
| 22:b:6022:CLA:C3D  | 22:b:6022:CLA:C20  | 2.88                     | 0.52              |
| 3:c:5146:PHE:C     | 3:c:5147:PHE:CG    | 2.85                     | 0.52              |
| 3:c:5223:TRP:NE1   | 3:c:5224:ILE:CG1   | 2.69                     | 0.52              |
| 3:c:5328:VAL:HG12  | 3:c:5340:TYR:HB2   | 1.91                     | 0.52              |
| 22:c:6028:CLA:H91  | 29:c:6056:DGD:CAB  | 2.36                     | 0.52              |
| 4:d:5182:LEU:N     | 4:d:5182:LEU:HD23  | 2.24                     | 0.52              |
| 4:d:5185:PHE:CE1   | 22:d:6004:CLA:HMD2 | 2.44                     | 0.52              |
| 24:d:6042:PQ9:H252 | 28:l:6061:MGE:H261 | 1.92                     | 0.52              |
| 13:o:5055:ALA:HA   | 13:o:5162:ILE:O    | 2.10                     | 0.52              |
| 13:o:5063:THR:CG2  | 13:o:5271:PRO:O    | 2.57                     | 0.52              |
| 15:u:5043:PRO:HB2  | 16:v:5109:ASP:HB2  | 1.91                     | 0.52              |
| 1:A:156:ALA:CB     | 1:A:160:ILE:HD12   | 2.40                     | 0.52              |
| 1:A:256:GLY:O      | 1:A:261:GLN:HA     | 2.10                     | 0.52              |
| 22:A:1006:CLA:CAB  | 22:D:1004:CLA:H51  | 2.37                     | 0.52              |
| 2:B:249:ALA:O      | 2:B:251:VAL:N      | 2.42                     | 0.52              |
| 22:B:1014:CLA:CHA  | 22:B:1014:CLA:CBA  | 2.78                     | 0.52              |
| 22:B:1022:CLA:C9   | 22:B:1022:CLA:C13  | 2.78                     | 0.52              |
| 22:B:1022:CLA:OBD  | 22:B:1022:CLA:CED  | 2.55                     | 0.52              |
| 3:C:62:PHE:CE2     | 10:K:29:PRO:HD3    | 2.45                     | 0.52              |
| 3:C:87:ILE:HG22    | 3:C:426:LEU:CD1    | 2.40                     | 0.52              |
| 25:T:6046:BCR:H351 | 25:b:6047:BCR:H23C | 1.92                     | 0.52              |
| 25:T:6048:BCR:H352 | 2:b:5106:LEU:HD12  | 1.91                     | 0.52              |
| 16:V:34:LEU:CD2    | 16:V:47:LEU:HB3    | 2.30                     | 0.52              |
| 16:V:160:LYS:N     | 16:V:163:TYR:CD1   | 2.78                     | 0.52              |
| 1:a:5156:ALA:CB    | 1:a:5160:ILE:HD12  | 2.40                     | 0.52              |
| 1:a:5214:MET:O     | 1:a:5217:SER:N     | 2.43                     | 0.52              |
| 1:a:5215:HIS:HE2   | 1:a:5272:HIS:CD2   | 2.28                     | 0.52              |
| 2:b:5026:HIS:NE2   | 22:b:6021:CLA:NB   | 2.57                     | 0.52              |
| 2:b:5363:PHE:HD2   | 2:b:5363:PHE:H     | 1.57                     | 0.52              |
| 2:b:5446:SER:O     | 2:b:5447:PRO:C     | 2.52                     | 0.52              |
| 3:c:5048:LYS:CG    | 3:c:5049:LEU:HD12  | 2.38                     | 0.52              |
| 3:c:5075:PHE:CZ    | 3:c:5105:VAL:HG11  | 2.37                     | 0.52              |
| 3:c:5117:VAL:HG21  | 22:c:6027:CLA:H43  | 1.90                     | 0.52              |
| 3:c:5158:THR:HG23  | 3:c:5159:THR:N     | 2.25                     | 0.52              |
| 4:d:5082:ALA:C     | 4:d:5084:SER:H     | 2.16                     | 0.52              |
| 25:h:6049:BCR:C23  | 25:h:6049:BCR:H393 | 2.30                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i:5008:VAL:O     | 8:i:5009:TYR:C     | 2.52                     | 0.52              |
| 13:o:5097:VAL:HG12 | 13:o:5098:THR:N    | 2.25                     | 0.52              |
| 13:o:5223:ILE:HG22 | 13:o:5243:SER:CB   | 2.36                     | 0.52              |
| 16:v:5108:TYR:HD2  | 16:v:5108:TYR:O    | 1.93                     | 0.52              |
| 1:A:272:HIS:O      | 4:D:215:GLY:CA     | 2.58                     | 0.52              |
| 1:A:279:ARG:NH2    | 1:A:283:VAL:CG2    | 2.73                     | 0.52              |
| 1:A:288:LEU:O      | 1:A:292:THR:N      | 2.42                     | 0.52              |
| 25:A:1044:BCR:H392 | 25:A:1044:BCR:C22  | 2.35                     | 0.52              |
| 2:B:5:TRP:CZ2      | 28:L:1061:MGE:C2A  | 2.80                     | 0.52              |
| 2:B:65:PHE:C       | 2:B:67:ALA:N       | 2.67                     | 0.52              |
| 2:B:203:ILE:HG23   | 2:B:204:ALA:N      | 2.24                     | 0.52              |
| 2:B:446:SER:O      | 2:B:447:PRO:C      | 2.52                     | 0.52              |
| 3:C:414:ILE:HG22   | 3:C:415:ASN:N      | 2.25                     | 0.52              |
| 25:D:1050:BCR:H331 | 25:D:1050:BCR:C8   | 2.28                     | 0.52              |
| 7:H:47:GLU:O       | 7:H:53:LEU:N       | 2.40                     | 0.52              |
| 15:U:43:PRO:HB2    | 16:V:109:ASP:HB2   | 1.91                     | 0.52              |
| 1:a:5180:PHE:O     | 1:a:5184:ILE:HD12  | 2.09                     | 0.52              |
| 2:b:5079:SER:OG    | 2:b:5080:ILE:N     | 2.41                     | 0.52              |
| 2:b:5111:ALA:C     | 2:b:5113:TRP:N     | 2.68                     | 0.52              |
| 2:b:5365:SER:O     | 2:b:5366:PHE:HB2   | 2.10                     | 0.52              |
| 2:b:5374:ASN:N     | 2:b:5374:ASN:ND2   | 2.58                     | 0.52              |
| 2:b:5425:ILE:O     | 2:b:5425:ILE:HG23  | 2.09                     | 0.52              |
| 3:c:5314:ALA:HB1   | 3:c:5351:PHE:CD1   | 2.45                     | 0.52              |
| 4:d:5251:ARG:NH2   | 4:d:5255:GLN:NE2   | 2.58                     | 0.52              |
| 5:e:5013:ILE:CD1   | 5:e:5019:TYR:HB2   | 2.40                     | 0.52              |
| 28:l:6061:MGE:H7B1 | 28:l:6061:MGE:H3B2 | 1.92                     | 0.52              |
| 13:o:5146:PHE:CE2  | 13:o:5261:ILE:HG21 | 2.43                     | 0.52              |
| 16:v:5092:ARG:CG   | 16:v:5092:ARG:NH1  | 2.67                     | 0.52              |
| 16:v:5160:LYS:N    | 16:v:5163:TYR:CD1  | 2.78                     | 0.52              |
| 16:v:5162:TYR:O    | 16:v:5163:TYR:C    | 2.53                     | 0.52              |
| 1:A:91:LEU:O       | 1:A:92:HIS:C       | 2.50                     | 0.52              |
| 2:B:215:PHE:C      | 2:B:215:PHE:CD2    | 2.88                     | 0.52              |
| 25:C:1052:BCR:C34  | 25:K:1051:BCR:HC21 | 2.39                     | 0.52              |
| 4:D:250:ASN:C      | 4:D:252:PHE:H      | 2.17                     | 0.52              |
| 5:E:59:GLU:OE1     | 5:E:59:GLU:HA      | 2.09                     | 0.52              |
| 6:F:32:PHE:O       | 6:F:32:PHE:HD1     | 1.93                     | 0.52              |
| 22:K:1034:CLA:H42  | 22:K:1034:CLA:HBA1 | 1.92                     | 0.52              |
| 13:O:82:PRO:HG2    | 13:O:89:ALA:HB1    | 1.87                     | 0.52              |
| 1:a:5219:VAL:HG11  | 4:d:5268:HIS:ND1   | 2.24                     | 0.52              |
| 1:a:5297:LEU:HD12  | 3:c:5428:THR:HG21  | 1.91                     | 0.52              |
| 22:b:6015:CLA:CBC  | 25:b:6047:BCR:H10C | 2.40                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5033:PHE:CZ    | 3:c:5040:ALA:HB1   | 2.45                     | 0.52              |
| 3:c:5296:VAL:HG23  | 3:c:5297:TYR:HD1   | 1.70                     | 0.52              |
| 4:d:5265:ARG:O     | 4:d:5265:ARG:HD3   | 2.10                     | 0.52              |
| 6:f:5032:PHE:O     | 6:f:5032:PHE:HD1   | 1.92                     | 0.52              |
| 7:h:5035:MET:HA    | 25:h:6049:BCR:C33  | 2.39                     | 0.52              |
| 11:l:5008:GLN:HE21 | 11:l:5008:GLN:N    | 2.07                     | 0.52              |
| 11:l:5023:LEU:O    | 11:l:5027:LEU:HG   | 2.09                     | 0.52              |
| 16:v:5119:PRO:CB   | 16:v:5130:MET:HE2  | 2.39                     | 0.52              |
| 1:A:37:MET:HE1     | 1:A:129:ARG:CZ     | 2.40                     | 0.52              |
| 1:A:58:VAL:HG21    | 1:A:83:VAL:HG23    | 1.91                     | 0.52              |
| 1:A:156:ALA:HB1    | 1:A:290:ILE:HG21   | 1.90                     | 0.52              |
| 2:B:19:LEU:O       | 2:B:22:ALA:HB3     | 2.10                     | 0.52              |
| 2:B:67:ALA:HB3     | 2:B:267:LEU:CD1    | 2.40                     | 0.52              |
| 2:B:365:SER:O      | 2:B:366:PHE:HB2    | 2.10                     | 0.52              |
| 2:B:413:ASP:O      | 2:B:413:ASP:OD1    | 2.28                     | 0.52              |
| 22:B:1016:CLA:O1A  | 22:B:1016:CLA:C1A  | 2.58                     | 0.52              |
| 22:B:1020:CLA:C16  | 22:B:1020:CLA:H111 | 2.39                     | 0.52              |
| 22:B:1021:CLA:HED3 | 22:B:1021:CLA:HMA3 | 1.91                     | 0.52              |
| 28:B:1060:MGE:H5A2 | 28:B:1060:MGE:H261 | 1.91                     | 0.52              |
| 3:C:171:GLY:C      | 3:C:174:LEU:H      | 2.18                     | 0.52              |
| 3:C:194:GLY:O      | 3:C:195:ASP:HB2    | 2.09                     | 0.52              |
| 3:C:200:THR:O      | 3:C:202:PRO:HD3    | 2.10                     | 0.52              |
| 4:D:55:VAL:HG12    | 4:D:56:THR:O       | 2.10                     | 0.52              |
| 4:D:78:VAL:HG12    | 4:D:173:PHE:CB     | 2.40                     | 0.52              |
| 4:D:88:SER:C       | 4:D:90:LEU:H       | 2.17                     | 0.52              |
| 22:D:1008:CLA:CBA  | 22:D:1008:CLA:HMA2 | 2.02                     | 0.52              |
| 7:H:27:THR:HB      | 22:H:1017:CLA:OBD  | 2.10                     | 0.52              |
| 13:O:215:ARG:HG2   | 13:O:215:ARG:NH1   | 2.24                     | 0.52              |
| 1:a:5156:ALA:HB1   | 1:a:5290:ILE:HG21  | 1.90                     | 0.52              |
| 1:a:5189:GLU:C     | 3:c:5411:ALA:HB2   | 2.35                     | 0.52              |
| 2:b:5015:ASP:OD2   | 2:b:5018:ARG:HG3   | 2.09                     | 0.52              |
| 2:b:5152:GLY:O     | 2:b:5156:PHE:CB    | 2.57                     | 0.52              |
| 2:b:5302:TRP:CE3   | 2:b:5305:ILE:HD12  | 2.45                     | 0.52              |
| 2:b:5463:PHE:CD2   | 2:b:5463:PHE:C     | 2.87                     | 0.52              |
| 22:b:6016:CLA:C9   | 22:d:6008:CLA:H201 | 2.40                     | 0.52              |
| 3:c:5062:PHE:CE2   | 10:k:5029:PRO:HD3  | 2.45                     | 0.52              |
| 3:c:5087:ILE:HG22  | 3:c:5426:LEU:CD1   | 2.40                     | 0.52              |
| 3:c:5135:ARG:NH1   | 20:z:5033:TRP:CE3  | 2.76                     | 0.52              |
| 3:c:5171:GLY:C     | 3:c:5174:LEU:H     | 2.18                     | 0.52              |
| 3:c:5405:ASN:OD1   | 29:c:6057:DGD:HD61 | 2.09                     | 0.52              |
| 4:d:5055:VAL:HG12  | 4:d:5056:THR:O     | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5198:MET:SD    | 22:d:6005:CLA:HED2 | 2.50                     | 0.52              |
| 5:e:5017:VAL:HG13  | 9:j:5008:ILE:HD11  | 1.91                     | 0.52              |
| 5:e:5023:HIS:HB3   | 5:e:5027:ILE:CD1   | 2.40                     | 0.52              |
| 13:o:5063:THR:HG23 | 13:o:5064:TYR:N    | 2.25                     | 0.52              |
| 16:v:5090:PRO:HD2  | 16:v:5092:ARG:CZ   | 2.40                     | 0.52              |
| 1:A:50:ILE:HG21    | 25:A:1044:BCR:H402 | 1.93                     | 0.51              |
| 1:A:92:HIS:CD2     | 3:C:219:GLY:O      | 2.64                     | 0.51              |
| 1:A:179:THR:O      | 1:A:180:PHE:C      | 2.52                     | 0.51              |
| 1:A:189:GLU:C      | 3:C:411:ALA:HB2    | 2.35                     | 0.51              |
| 2:B:142:HIS:HA     | 2:B:145:LEU:HD12   | 1.92                     | 0.51              |
| 2:B:475:PHE:C      | 2:B:477:ASP:H      | 2.16                     | 0.51              |
| 3:C:79:LYS:HD3     | 3:C:84:GLN:HG2     | 1.92                     | 0.51              |
| 22:C:1027:CLA:HAA1 | 22:C:1027:CLA:HBD  | 1.92                     | 0.51              |
| 4:D:23:LYS:NZ      | 4:D:135:LEU:HD21   | 2.25                     | 0.51              |
| 4:D:251:ARG:NH2    | 4:D:255:GLN:NE2    | 2.58                     | 0.51              |
| 4:D:267:LEU:C      | 4:D:269:PHE:H      | 2.18                     | 0.51              |
| 4:D:308:ASP:C      | 4:D:310:GLU:H      | 2.17                     | 0.51              |
| 5:E:13:ILE:HA      | 5:E:16:SER:HB3     | 1.92                     | 0.51              |
| 5:E:28:PRO:HA      | 5:E:31:PHE:HB3     | 1.92                     | 0.51              |
| 10:K:31:LEU:HD13   | 25:K:1051:BCR:H14C | 1.91                     | 0.51              |
| 22:K:1034:CLA:CHD  | 22:K:1034:CLA:CBC  | 2.84                     | 0.51              |
| 13:O:55:ALA:HA     | 13:O:162:ILE:O     | 2.10                     | 0.51              |
| 1:a:5201:GLY:C     | 1:a:5203:ALA:N     | 2.65                     | 0.51              |
| 1:a:5333:GLU:OE1   | 3:c:5354:GLU:OE1   | 2.28                     | 0.51              |
| 2:b:5249:ALA:O     | 2:b:5251:VAL:N     | 2.42                     | 0.51              |
| 2:b:5256:MET:HE1   | 2:b:5268:PHE:CE2   | 2.45                     | 0.51              |
| 22:b:6010:CLA:H151 | 29:b:6058:DGD:C8A  | 2.38                     | 0.51              |
| 22:b:6019:CLA:HMA2 | 22:b:6020:CLA:CMC  | 2.39                     | 0.51              |
| 25:b:6047:BCR:H403 | 25:b:6047:BCR:C22  | 2.34                     | 0.51              |
| 3:c:5056:HIS:CE1   | 22:c:6033:CLA:HHB  | 2.44                     | 0.51              |
| 3:c:5271:TYR:CE1   | 22:c:6031:CLA:CAC  | 2.83                     | 0.51              |
| 3:c:5414:ILE:HG22  | 3:c:5415:ASN:N     | 2.25                     | 0.51              |
| 22:c:6035:CLA:HBD  | 22:c:6035:CLA:HAA1 | 1.92                     | 0.51              |
| 5:e:5072:ALA:O     | 5:e:5076:VAL:HG22  | 2.11                     | 0.51              |
| 15:u:5016:LYS:NZ   | 15:u:5085:THR:HB   | 2.25                     | 0.51              |
| 1:A:86:SER:C       | 1:A:88:ALA:H       | 2.18                     | 0.51              |
| 1:A:180:PHE:O      | 1:A:184:ILE:HD12   | 2.09                     | 0.51              |
| 2:B:111:ALA:C      | 2:B:113:TRP:N      | 2.68                     | 0.51              |
| 2:B:192:PRO:HD2    | 7:H:60:VAL:HG12    | 1.92                     | 0.51              |
| 2:B:310:ALA:O      | 2:B:313:ASP:N      | 2.41                     | 0.51              |
| 2:B:362:PHE:HZ     | 27:D:1068:IOD:I    | 2.63                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1015:CLA:CB   | 25:B:1047:BCR:H10C | 2.40                     | 0.51              |
| 22:B:1019:CLA:H93  | 28:L:1061:MGE:C8A  | 2.41                     | 0.51              |
| 22:B:1022:CLA:C3D  | 22:B:1022:CLA:C20  | 2.88                     | 0.51              |
| 3:C:33:PHE:CZ      | 3:C:40:ALA:HB1     | 2.45                     | 0.51              |
| 22:C:1035:CLA:HBD  | 22:C:1035:CLA:HAA1 | 1.92                     | 0.51              |
| 25:C:1054:BCR:H23C | 25:C:1054:BCR:H402 | 1.73                     | 0.51              |
| 4:D:274:VAL:HG12   | 4:D:275:PRO:N      | 2.24                     | 0.51              |
| 8:I:27:ASP:N       | 8:I:28:PRO:CD      | 2.74                     | 0.51              |
| 13:O:148:VAL:HG23  | 13:O:151:LEU:HD13  | 1.92                     | 0.51              |
| 15:U:45:LEU:HD21   | 15:U:75:LEU:HD11   | 1.92                     | 0.51              |
| 1:a:5037:MET:O     | 1:a:5038:ILE:C     | 2.51                     | 0.51              |
| 1:a:5050:ILE:HG21  | 25:a:6044:BCR:H402 | 1.92                     | 0.51              |
| 1:a:5081:ALA:HA    | 1:a:5175:GLY:HA3   | 1.92                     | 0.51              |
| 1:a:5146:ALA:HA    | 1:a:5280:VAL:HG11  | 1.91                     | 0.51              |
| 1:a:5148:SER:OG    | 1:a:5149:ALA:N     | 2.43                     | 0.51              |
| 2:b:5019:LEU:O     | 2:b:5022:ALA:HB3   | 2.09                     | 0.51              |
| 2:b:5271:THR:O     | 2:b:5274:GLN:HB2   | 2.10                     | 0.51              |
| 2:b:5413:ASP:OD1   | 2:b:5413:ASP:O     | 2.28                     | 0.51              |
| 22:b:6010:CLA:H112 | 22:b:6010:CLA:C17  | 2.36                     | 0.51              |
| 22:b:6019:CLA:HBB1 | 22:b:6019:CLA:CHC  | 2.37                     | 0.51              |
| 3:c:5079:LYS:HD3   | 3:c:5084:GLN:HG2   | 1.92                     | 0.51              |
| 3:c:5275:SER:C     | 22:c:6033:CLA:HED1 | 2.35                     | 0.51              |
| 22:c:6027:CLA:HBC3 | 22:c:6027:CLA:CMC  | 2.39                     | 0.51              |
| 7:h:5027:THR:HB    | 22:h:6017:CLA:OBD  | 2.10                     | 0.51              |
| 22:k:6034:CLA:H42  | 22:k:6034:CLA:CBA  | 2.41                     | 0.51              |
| 12:m:5011:THR:O    | 12:m:5014:PHE:HB3  | 2.10                     | 0.51              |
| 13:o:5137:ALA:O    | 13:o:5138:GLY:O    | 2.28                     | 0.51              |
| 14:t:5011:ALA:CB   | 25:t:1046:BCR:H362 | 2.40                     | 0.51              |
| 15:u:5044:THR:O    | 15:u:5045:LEU:C    | 2.51                     | 0.51              |
| 1:A:75:ASN:HD22    | 1:A:80:GLY:HA2     | 1.76                     | 0.51              |
| 1:A:107:TYR:CD2    | 13:O:97:VAL:HG11   | 2.44                     | 0.51              |
| 1:A:180:PHE:CZ     | 4:D:192:THR:O      | 2.63                     | 0.51              |
| 1:A:279:ARG:CZ     | 1:A:283:VAL:HG22   | 2.40                     | 0.51              |
| 1:A:335:ASN:OD1    | 1:A:335:ASN:N      | 2.43                     | 0.51              |
| 22:A:1006:CLA:HAA2 | 29:C:1057:DGD:CFB  | 2.40                     | 0.51              |
| 2:B:14:ASN:O       | 2:B:15:ASP:HB3     | 2.09                     | 0.51              |
| 2:B:30:VAL:CG1     | 22:B:1013:CLA:HHD  | 2.40                     | 0.51              |
| 2:B:61:PHE:HB2     | 22:B:1015:CLA:HMA1 | 1.93                     | 0.51              |
| 2:B:125:ASP:HA     | 7:H:12:ARG:HH21    | 1.75                     | 0.51              |
| 2:B:302:TRP:C      | 2:B:304:ALA:N      | 2.66                     | 0.51              |
| 3:C:72:LEU:HD22    | 10:K:11:LEU:HD23   | 1.91                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:126:MET:CE     | 4:D:146:PHE:HB3    | 2.40                     | 0.51              |
| 4:D:214:HIS:CE1    | 4:D:268:HIS:CE1    | 2.98                     | 0.51              |
| 5:E:72:ALA:O       | 5:E:76:VAL:HG22    | 2.11                     | 0.51              |
| 11:L:26:VAL:O      | 11:L:29:LEU:N      | 2.43                     | 0.51              |
| 1:a:5310:LYS:H     | 16:v:5028:GLU:HB2  | 1.76                     | 0.51              |
| 2:b:5005:TRP:CD1   | 2:b:5005:TRP:N     | 2.76                     | 0.51              |
| 2:b:5024:LEU:HB2   | 22:b:6023:CLA:HED1 | 1.92                     | 0.51              |
| 2:b:5065:PHE:HZ    | 22:b:6012:CLA:HMA3 | 1.72                     | 0.51              |
| 3:c:5318:LEU:HD11  | 3:c:5380:ILE:HG12  | 1.92                     | 0.51              |
| 4:d:5264:LYS:HB3   | 4:d:5268:HIS:CE1   | 2.45                     | 0.51              |
| 8:i:5027:ASP:N     | 8:i:5028:PRO:CD    | 2.74                     | 0.51              |
| 9:j:5008:ILE:H     | 9:j:5008:ILE:HD12  | 1.76                     | 0.51              |
| 9:j:5020:GLY:O     | 9:j:5023:VAL:HG12  | 2.09                     | 0.51              |
| 15:u:5058:VAL:HB   | 15:u:5059:GLU:OE2  | 2.11                     | 0.51              |
| 16:v:5151:ILE:HD13 | 16:v:5151:ILE:N    | 2.23                     | 0.51              |
| 1:A:37:MET:HE1     | 1:A:129:ARG:NH2    | 2.26                     | 0.51              |
| 1:A:151:LEU:HG     | 1:A:155:PHE:CD2    | 2.44                     | 0.51              |
| 1:A:310:LYS:H      | 16:V:28:GLU:HB2    | 1.76                     | 0.51              |
| 26:A:1063:LHG:C31  | 22:C:1032:CLA:H71  | 2.41                     | 0.51              |
| 2:B:99:ALA:O       | 2:B:102:VAL:CG2    | 2.59                     | 0.51              |
| 2:B:121:GLU:CG     | 7:H:12:ARG:HD3     | 2.40                     | 0.51              |
| 2:B:152:GLY:O      | 2:B:156:PHE:CB     | 2.57                     | 0.51              |
| 2:B:256:MET:HE1    | 2:B:268:PHE:CE2    | 2.45                     | 0.51              |
| 22:B:1013:CLA:CMB  | 22:B:1014:CLA:C1   | 2.88                     | 0.51              |
| 28:B:1060:MGE:H6B1 | 4:D:280:TRP:CD1    | 2.46                     | 0.51              |
| 3:C:229:ASN:N      | 3:C:229:ASN:ND2    | 2.44                     | 0.51              |
| 22:C:1026:CLA:C2B  | 22:C:1028:CLA:CBB  | 2.88                     | 0.51              |
| 4:D:118:GLY:HA2    | 23:D:1039:PHO:H71  | 1.93                     | 0.51              |
| 4:D:126:MET:HE3    | 4:D:146:PHE:CD2    | 2.42                     | 0.51              |
| 4:D:154:VAL:HA     | 4:D:158:LEU:HD13   | 1.92                     | 0.51              |
| 4:D:167:TRP:O      | 4:D:170:ALA:HB3    | 2.10                     | 0.51              |
| 4:D:186:GLN:H      | 22:D:1004:CLA:HBC1 | 1.75                     | 0.51              |
| 4:D:188:PHE:CE2    | 4:D:326:ARG:HA     | 2.46                     | 0.51              |
| 1:a:5029:TYR:H     | 4:d:5255:GLN:HB3   | 1.75                     | 0.51              |
| 1:a:5120:LEU:HD11  | 1:a:5155:PHE:CE1   | 2.46                     | 0.51              |
| 1:a:5151:LEU:HG    | 1:a:5155:PHE:CD2   | 2.44                     | 0.51              |
| 22:a:6007:CLA:H43  | 22:c:6029:CLA:H192 | 1.89                     | 0.51              |
| 2:b:5025:MET:HG3   | 25:b:6045:BCR:C39  | 2.38                     | 0.51              |
| 3:c:5315:MET:O     | 3:c:5319:ILE:HG13  | 2.10                     | 0.51              |
| 22:c:6026:CLA:C2B  | 22:c:6028:CLA:CBB  | 2.88                     | 0.51              |
| 22:c:6029:CLA:H11  | 22:c:6029:CLA:CHA  | 2.39                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5067:TYR:CD1   | 4:d:5076:VAL:HG11  | 2.46                     | 0.51              |
| 4:d:5189:HIS:O     | 4:d:5190:ASN:C     | 2.52                     | 0.51              |
| 4:d:5249:ALA:HB1   | 24:d:6042:PQ9:C6   | 2.39                     | 0.51              |
| 24:d:6042:PQ9:C24  | 28:l:6061:MGE:CGB  | 2.81                     | 0.51              |
| 5:e:5013:ILE:HA    | 5:e:5016:SER:HB3   | 1.92                     | 0.51              |
| 5:e:5084:LYS:NZ    | 16:v:5027:ALA:O    | 2.43                     | 0.51              |
| 8:i:5011:VAL:O     | 8:i:5015:PHE:CD1   | 2.64                     | 0.51              |
| 10:k:5021:LEU:HD21 | 18:y:5024:MET:HE3  | 1.93                     | 0.51              |
| 10:k:5031:LEU:HD13 | 25:k:6051:BCR:H14C | 1.91                     | 0.51              |
| 11:l:5026:VAL:O    | 11:l:5029:LEU:N    | 2.44                     | 0.51              |
| 18:y:5032:GLY:O    | 18:y:5035:ILE:CG2  | 2.53                     | 0.51              |
| 1:A:17:PHE:O       | 1:A:21:VAL:HG23    | 2.10                     | 0.51              |
| 1:A:81:ALA:HA      | 1:A:175:GLY:HA3    | 1.92                     | 0.51              |
| 1:A:181:ASN:HD22   | 4:D:314:PHE:HD2    | 1.56                     | 0.51              |
| 1:A:331:MET:HA     | 1:A:331:MET:HE3    | 1.91                     | 0.51              |
| 2:B:368:VAL:HG22   | 2:B:381:ILE:HG13   | 1.93                     | 0.51              |
| 22:B:1022:CLA:HBC1 | 12:M:21:PHE:CG     | 2.46                     | 0.51              |
| 3:C:109:PHE:HB3    | 3:C:110:PRO:CD     | 2.40                     | 0.51              |
| 3:C:206:PRO:HG2    | 3:C:207:ARG:NH1    | 2.26                     | 0.51              |
| 3:C:290:VAL:HG13   | 3:C:427:ALA:HB2    | 1.93                     | 0.51              |
| 22:C:1028:CLA:H91  | 29:C:1056:DGD:CAB  | 2.36                     | 0.51              |
| 22:C:1028:CLA:C10  | 29:C:1056:DGD:HAS2 | 2.36                     | 0.51              |
| 22:C:1030:CLA:H171 | 22:C:1030:CLA:C14  | 2.21                     | 0.51              |
| 4:D:198:MET:SD     | 22:D:1005:CLA:HED2 | 2.50                     | 0.51              |
| 28:D:1062:MGE:O1B  | 28:D:1062:MGE:C3G  | 2.34                     | 0.51              |
| 22:K:1034:CLA:H42  | 22:K:1034:CLA:CBA  | 2.41                     | 0.51              |
| 28:L:1061:MGE:H7B1 | 28:L:1061:MGE:H3B2 | 1.92                     | 0.51              |
| 13:O:63:THR:HG23   | 13:O:64:TYR:N      | 2.25                     | 0.51              |
| 14:T:19:PHE:CD2    | 14:T:19:PHE:N      | 2.77                     | 0.51              |
| 25:T:6048:BCR:H392 | 25:T:6048:BCR:C22  | 2.35                     | 0.51              |
| 20:Z:20:VAL:HG12   | 20:Z:21:ILE:N      | 2.26                     | 0.51              |
| 20:Z:23:VAL:HB     | 20:Z:24:PRO:HD3    | 1.91                     | 0.51              |
| 1:a:5076:ASN:HB2   | 1:a:5079:THR:HG23  | 1.91                     | 0.51              |
| 1:a:5086:SER:C     | 1:a:5088:ALA:H     | 2.18                     | 0.51              |
| 1:a:5325:ASN:ND2   | 1:a:5328:MET:CE    | 2.73                     | 0.51              |
| 2:b:5354:LEU:CD2   | 2:b:5378:LYS:HB2   | 2.40                     | 0.51              |
| 22:b:6018:CLA:H8   | 22:b:6023:CLA:HBA1 | 1.90                     | 0.51              |
| 29:b:6058:DGD:CIB  | 29:b:6058:DGD:CEB  | 2.39                     | 0.51              |
| 3:c:5263:ALA:HB1   | 3:c:5264:PHE:CD2   | 2.45                     | 0.51              |
| 4:d:5261:PHE:H     | 24:d:6042:PQ9:H93  | 1.74                     | 0.51              |
| 6:f:5032:PHE:CD1   | 6:f:5032:PHE:C     | 2.87                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5150:ASN:HD22 | 13:o:5173:ASN:CB   | 2.24                     | 0.51              |
| 16:v:5039:ASN:C    | 16:v:5041:GLU:N    | 2.67                     | 0.51              |
| 1:A:45:THR:CG2     | 1:A:46:ILE:N       | 2.71                     | 0.51              |
| 1:A:149:ALA:HB3    | 1:A:150:PRO:CD     | 2.36                     | 0.51              |
| 1:A:265:PHE:CD1    | 1:A:271:LEU:HA     | 2.46                     | 0.51              |
| 2:B:325:PHE:O      | 2:B:327:THR:N      | 2.37                     | 0.51              |
| 29:B:1058:DGD:HE5  | 29:B:1058:DGD:HD61 | 1.93                     | 0.51              |
| 3:C:171:GLY:CA     | 3:C:174:LEU:CB     | 2.86                     | 0.51              |
| 3:C:202:PRO:HB3    | 3:C:235:GLY:CA     | 2.40                     | 0.51              |
| 4:D:67:TYR:CD1     | 4:D:76:VAL:HG11    | 2.46                     | 0.51              |
| 22:D:1008:CLA:C18  | 22:D:1008:CLA:H141 | 2.19                     | 0.51              |
| 16:V:162:TYR:O     | 16:V:163:TYR:C     | 2.53                     | 0.51              |
| 1:a:5037:MET:HE1   | 1:a:5129:ARG:NH2   | 2.26                     | 0.51              |
| 1:a:5064:ARG:HH21  | 13:o:5098:THR:HG21 | 1.76                     | 0.51              |
| 1:a:5256:GLY:O     | 1:a:5261:GLN:HA    | 2.10                     | 0.51              |
| 2:b:5095:GLY:O     | 2:b:5099:ALA:N     | 2.41                     | 0.51              |
| 2:b:5125:ASP:HA    | 7:h:5012:ARG:HH21  | 1.75                     | 0.51              |
| 2:b:5302:TRP:C     | 2:b:5304:ALA:N     | 2.66                     | 0.51              |
| 2:b:5372:ASP:OD2   | 2:b:5376:VAL:HG23  | 2.10                     | 0.51              |
| 22:b:6016:CLA:O1A  | 22:b:6016:CLA:C1A  | 2.58                     | 0.51              |
| 22:b:6016:CLA:CGA  | 22:b:6016:CLA:C1A  | 2.88                     | 0.51              |
| 3:c:5167:VAL:CG1   | 3:c:5168:LEU:HD12  | 2.30                     | 0.51              |
| 3:c:5171:GLY:O     | 3:c:5172:ALA:C     | 2.52                     | 0.51              |
| 22:c:6027:CLA:HBD  | 22:c:6027:CLA:HAA1 | 1.92                     | 0.51              |
| 4:d:5023:LYS:NZ    | 4:d:5135:LEU:HD21  | 2.26                     | 0.51              |
| 4:d:5078:VAL:HG12  | 4:d:5173:PHE:CB    | 2.40                     | 0.51              |
| 6:f:5038:ALA:HA    | 9:j:5027:LEU:HD21  | 1.91                     | 0.51              |
| 8:i:5029:ALA:O     | 8:i:5030:ARG:CB    | 2.59                     | 0.51              |
| 22:k:6034:CLA:C4D  | 22:k:6034:CLA:O2A  | 2.59                     | 0.51              |
| 2:B:99:ALA:O       | 2:B:102:VAL:HG22   | 2.11                     | 0.51              |
| 2:B:283:GLU:HG2    | 2:B:286:ARG:HH12   | 1.76                     | 0.51              |
| 3:C:171:GLY:C      | 22:C:1025:CLA:HBC3 | 2.35                     | 0.51              |
| 4:D:213:ILE:HD11   | 4:D:253:TRP:CH2    | 2.46                     | 0.51              |
| 4:D:246:MET:HE2    | 4:D:264:LYS:HD3    | 1.93                     | 0.51              |
| 7:H:56:ASP:C       | 7:H:58:VAL:N       | 2.63                     | 0.51              |
| 8:I:7:THR:O        | 8:I:11:VAL:HG23    | 2.11                     | 0.51              |
| 1:a:5149:ALA:HB3   | 1:a:5150:PRO:CD    | 2.36                     | 0.51              |
| 2:b:5192:PRO:HD2   | 7:h:5060:VAL:HG12  | 1.92                     | 0.51              |
| 13:o:5148:VAL:HG23 | 13:o:5151:LEU:HD13 | 1.92                     | 0.51              |
| 13:o:5176:SER:O    | 13:o:5177:TYR:C    | 2.54                     | 0.51              |
| 1:A:26:ASN:O       | 1:A:28:LEU:N       | 2.44                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:148:SER:OG     | 1:A:149:ALA:N      | 2.43                     | 0.51              |
| 1:A:269:ARG:CZ     | 4:D:222:LEU:CD2    | 2.89                     | 0.51              |
| 1:A:310:LYS:H      | 16:V:28:GLU:CB     | 2.24                     | 0.51              |
| 1:A:325:ASN:ND2    | 1:A:328:MET:CE     | 2.73                     | 0.51              |
| 24:A:1043:PQ9:H293 | 23:D:1039:PHO:HBA2 | 1.91                     | 0.51              |
| 2:B:27:THR:HG23    | 22:B:1013:CLA:HBC3 | 1.93                     | 0.51              |
| 2:B:271:THR:O      | 2:B:274:GLN:HB2    | 2.11                     | 0.51              |
| 22:B:1011:CLA:OBD  | 22:B:1013:CLA:H12  | 2.10                     | 0.51              |
| 3:C:274:TYR:CE1    | 22:C:1029:CLA:O1D  | 2.62                     | 0.51              |
| 22:C:1028:CLA:NB   | 29:C:1056:DGD:HA42 | 2.26                     | 0.51              |
| 22:C:1035:CLA:H93  | 25:C:1052:BCR:H402 | 1.87                     | 0.51              |
| 4:D:122:LEU:O      | 4:D:123:ILE:C      | 2.54                     | 0.51              |
| 4:D:274:VAL:HG13   | 24:D:1042:PQ9:H262 | 1.93                     | 0.51              |
| 10:K:21:LEU:HD21   | 18:Y:24:MET:HE3    | 1.92                     | 0.51              |
| 20:Z:12:LEU:HA     | 20:Z:50:LEU:HD13   | 1.93                     | 0.51              |
| 1:a:5269:ARG:CZ    | 4:d:5222:LEU:CD2   | 2.89                     | 0.51              |
| 1:a:5271:LEU:HD12  | 1:a:5272:HIS:N     | 2.26                     | 0.51              |
| 2:b:5060:MET:HE2   | 2:b:5060:MET:HA    | 1.93                     | 0.51              |
| 2:b:5275:TRP:HB3   | 2:b:5318:ASN:HD22  | 1.75                     | 0.51              |
| 22:b:6010:CLA:HBD  | 22:b:6010:CLA:HAA2 | 1.93                     | 0.51              |
| 22:b:6019:CLA:HBB2 | 22:b:6021:CLA:CMB  | 2.41                     | 0.51              |
| 3:c:5117:VAL:CG1   | 22:c:6027:CLA:H42  | 2.32                     | 0.51              |
| 4:d:5118:GLY:HA2   | 23:d:6039:PHO:H71  | 1.93                     | 0.51              |
| 4:d:5126:MET:HE3   | 4:d:5146:PHE:CD2   | 2.42                     | 0.51              |
| 22:d:6005:CLA:O1A  | 22:d:6005:CLA:NA   | 2.43                     | 0.51              |
| 10:k:5032:PHE:HB3  | 22:k:6034:CLA:HMA3 | 1.91                     | 0.51              |
| 13:o:5154:SER:O    | 13:o:5168:PHE:HA   | 2.11                     | 0.51              |
| 16:v:5058:LEU:O    | 16:v:5060:GLN:N    | 2.44                     | 0.51              |
| 1:A:115:ILE:HG21   | 1:A:174:LEU:HD13   | 1.93                     | 0.51              |
| 1:A:333:GLU:OE1    | 3:C:354:GLU:OE1    | 2.28                     | 0.51              |
| 2:B:24:LEU:HB2     | 22:B:1023:CLA:HED1 | 1.92                     | 0.51              |
| 2:B:24:LEU:HD22    | 2:B:114:HIS:HD2    | 1.75                     | 0.51              |
| 2:B:338:GLN:HA     | 2:B:338:GLN:NE2    | 2.16                     | 0.51              |
| 22:B:1016:CLA:C1A  | 22:B:1016:CLA:CGA  | 2.88                     | 0.51              |
| 3:C:158:THR:HG23   | 3:C:159:THR:N      | 2.25                     | 0.51              |
| 3:C:275:SER:C      | 22:C:1033:CLA:HED1 | 2.35                     | 0.51              |
| 5:E:23:HIS:HB3     | 5:E:27:ILE:CD1     | 2.40                     | 0.51              |
| 7:H:38:PHE:O       | 7:H:41:PHE:N       | 2.41                     | 0.51              |
| 8:I:8:VAL:O        | 8:I:9:TYR:C        | 2.52                     | 0.51              |
| 8:I:11:VAL:O       | 8:I:15:PHE:CD1     | 2.64                     | 0.51              |
| 10:K:20:PRO:O      | 10:K:23:ASP:HB2    | 2.11                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:K:1034:CLA:C4D  | 22:K:1034:CLA:O2A  | 2.59                     | 0.51              |
| 13:O:176:SER:O     | 13:O:177:TYR:C     | 2.54                     | 0.51              |
| 14:T:11:ALA:O      | 14:T:13:ILE:N      | 2.44                     | 0.51              |
| 16:V:58:LEU:O      | 16:V:60:GLN:N      | 2.44                     | 0.51              |
| 1:a:5033:PHE:O     | 1:a:5034:GLY:C     | 2.54                     | 0.51              |
| 1:a:5037:MET:HE1   | 1:a:5129:ARG:CZ    | 2.40                     | 0.51              |
| 1:a:5147:TYR:O     | 1:a:5150:PRO:HD2   | 2.11                     | 0.51              |
| 1:a:5272:HIS:O     | 4:d:5215:GLY:HA2   | 2.11                     | 0.51              |
| 22:a:6006:CLA:HAA2 | 29:c:6057:DGD:CFB  | 2.40                     | 0.51              |
| 22:a:6007:CLA:H142 | 8:i:5013:THR:HG21  | 1.92                     | 0.51              |
| 26:a:6063:LHG:C31  | 22:c:6032:CLA:H71  | 2.41                     | 0.51              |
| 2:b:5014:ASN:O     | 2:b:5015:ASP:HB3   | 2.09                     | 0.51              |
| 2:b:5142:HIS:HA    | 2:b:5145:LEU:HD12  | 1.92                     | 0.51              |
| 22:b:6011:CLA:C1D  | 22:b:6013:CLA:C4   | 2.89                     | 0.51              |
| 22:b:6012:CLA:HMD2 | 22:b:6020:CLA:H201 | 1.92                     | 0.51              |
| 22:b:6019:CLA:H93  | 28:l:6061:MGE:C8A  | 2.41                     | 0.51              |
| 22:b:6022:CLA:HBC1 | 12:m:5021:PHE:CG   | 2.46                     | 0.51              |
| 22:c:6028:CLA:NB   | 29:c:6056:DGD:HA42 | 2.26                     | 0.51              |
| 4:d:5037:LEU:CD1   | 4:d:5125:PHE:HB2   | 2.41                     | 0.51              |
| 4:d:5154:VAL:HA    | 4:d:5158:LEU:HD13  | 1.92                     | 0.51              |
| 4:d:5188:PHE:CE2   | 4:d:5326:ARG:HA    | 2.46                     | 0.51              |
| 4:d:5274:VAL:HG13  | 24:d:6042:PQ9:H262 | 1.93                     | 0.51              |
| 4:d:5331:PRO:HA    | 4:d:5339:PHE:HB2   | 1.92                     | 0.51              |
| 22:d:6008:CLA:HBB1 | 22:d:6008:CLA:CHC  | 2.13                     | 0.51              |
| 24:d:6042:PQ9:H252 | 28:l:6061:MGE:CGB  | 2.41                     | 0.51              |
| 5:e:5028:PRO:HA    | 5:e:5031:PHE:HB3   | 1.92                     | 0.51              |
| 11:l:5015:THR:HG22 | 11:l:5016:SER:N    | 2.22                     | 0.51              |
| 16:v:5061:TYR:C    | 16:v:5063:CYS:N    | 2.68                     | 0.51              |
| 17:x:5036:VAL:O    | 17:x:5039:ALA:HB3  | 2.10                     | 0.51              |
| 20:z:5023:VAL:HB   | 20:z:5024:PRO:HD3  | 1.91                     | 0.51              |
| 1:A:41:LEU:O       | 1:A:45:THR:HG22    | 2.11                     | 0.51              |
| 1:A:76:ASN:HB2     | 4:D:298:PHE:HE1    | 1.76                     | 0.51              |
| 1:A:143:ILE:HD11   | 4:D:253:TRP:CZ2    | 2.46                     | 0.51              |
| 1:A:216:GLY:HA2    | 4:D:268:HIS:O      | 2.11                     | 0.51              |
| 1:A:338:ASN:O      | 1:A:339:PHE:CD2    | 2.64                     | 0.51              |
| 2:B:74:SER:O       | 2:B:76:SER:N       | 2.44                     | 0.51              |
| 2:B:109:LEU:O      | 2:B:110:ALA:C      | 2.54                     | 0.51              |
| 2:B:302:TRP:CE3    | 2:B:305:ILE:HD12   | 2.45                     | 0.51              |
| 22:B:1010:CLA:O2D  | 22:B:1010:CLA:H2A  | 2.11                     | 0.51              |
| 22:B:1016:CLA:C9   | 22:D:1008:CLA:H201 | 2.40                     | 0.51              |
| 22:B:1018:CLA:HHC  | 22:B:1018:CLA:CBB  | 2.20                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B:1047:BCR:H23C | 25:t:1046:BCR:H351 | 1.92                     | 0.51              |
| 3:C:48:LYS:CG      | 3:C:49:LEU:HD12    | 2.38                     | 0.51              |
| 3:C:185:LEU:CG     | 3:C:199:ILE:HD11   | 2.38                     | 0.51              |
| 3:C:223:TRP:CD1    | 3:C:223:TRP:C      | 2.89                     | 0.51              |
| 3:C:318:LEU:HD11   | 3:C:380:ILE:HG12   | 1.92                     | 0.51              |
| 5:E:73:LYS:O       | 5:E:76:VAL:CG2     | 2.54                     | 0.51              |
| 5:E:84:LYS:NZ      | 16:V:27:ALA:O      | 2.43                     | 0.51              |
| 12:M:18:PRO:HG2    | 12:M:19:SER:N      | 2.26                     | 0.51              |
| 12:M:18:PRO:O      | 12:M:21:PHE:HB3    | 2.11                     | 0.51              |
| 13:O:80:GLU:HB2    | 13:O:92:VAL:HG23   | 1.93                     | 0.51              |
| 16:V:90:PRO:HD2    | 16:V:92:ARG:CZ     | 2.40                     | 0.51              |
| 16:V:119:PRO:HB2   | 16:V:130:MET:HE2   | 1.92                     | 0.51              |
| 1:a:5041:LEU:O     | 1:a:5045:THR:HG22  | 2.11                     | 0.51              |
| 1:a:5202:VAL:HG22  | 1:a:5206:PHE:CD1   | 2.46                     | 0.51              |
| 1:a:5210:LEU:C     | 1:a:5210:LEU:CD2   | 2.84                     | 0.51              |
| 1:a:5215:HIS:O     | 1:a:5219:VAL:HG23  | 2.11                     | 0.51              |
| 1:a:5265:PHE:CD1   | 1:a:5271:LEU:HA    | 2.46                     | 0.51              |
| 1:a:5279:ARG:HE    | 23:a:6038:PHO:HMC3 | 1.76                     | 0.51              |
| 2:b:5027:THR:HG23  | 22:b:6013:CLA:HBC3 | 1.93                     | 0.51              |
| 2:b:5065:PHE:C     | 2:b:5067:ALA:N     | 2.67                     | 0.51              |
| 2:b:5190:PHE:CZ    | 22:b:6009:CLA:HMA1 | 2.45                     | 0.51              |
| 2:b:5434:THR:OG1   | 13:o:5204:LYS:HD3  | 2.11                     | 0.51              |
| 3:c:5062:PHE:CZ    | 10:k:5028:ILE:HB   | 2.46                     | 0.51              |
| 3:c:5348:GLU:H     | 13:o:5042:ALA:HB3  | 1.76                     | 0.51              |
| 4:d:5029:PHE:CD2   | 4:d:5030:VAL:N     | 2.79                     | 0.51              |
| 4:d:5033:SER:OG    | 4:d:5128:ARG:HG3   | 2.11                     | 0.51              |
| 4:d:5167:TRP:O     | 4:d:5170:ALA:HB3   | 2.10                     | 0.51              |
| 8:i:5007:THR:O     | 8:i:5011:VAL:HG23  | 2.11                     | 0.51              |
| 10:k:5033:PHE:CE1  | 10:k:5037:PHE:CE2  | 2.98                     | 0.51              |
| 12:m:5018:PRO:HG2  | 12:m:5019:SER:N    | 2.26                     | 0.51              |
| 1:A:29:TYR:H       | 4:D:255:GLN:HB3    | 1.75                     | 0.50              |
| 1:A:64:ARG:HH21    | 13:O:98:THR:HG21   | 1.76                     | 0.50              |
| 1:A:76:ASN:HB2     | 1:A:79:THR:HG23    | 1.91                     | 0.50              |
| 2:B:21:ALA:HA      | 2:B:24:LEU:HD23    | 1.94                     | 0.50              |
| 2:B:340:TRP:HE1    | 2:B:428:GLU:HB3    | 1.76                     | 0.50              |
| 2:B:467:ILE:HD13   | 4:D:126:MET:SD     | 2.52                     | 0.50              |
| 3:C:251:HIS:HE1    | 22:C:1030:CLA:NA   | 2.09                     | 0.50              |
| 22:D:1005:CLA:HBC2 | 22:D:1005:CLA:CHD  | 2.41                     | 0.50              |
| 7:H:43:LEU:CD2     | 17:X:19:PHE:CZ     | 2.92                     | 0.50              |
| 13:O:97:VAL:HG12   | 13:O:98:THR:N      | 2.25                     | 0.50              |
| 13:O:137:ALA:O     | 13:O:138:GLY:O     | 2.28                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:T:22:PHE:N      | 14:T:22:PHE:CD1    | 2.79                     | 0.50              |
| 25:T:6046:BCR:H353 | 25:b:6047:BCR:C23  | 2.41                     | 0.50              |
| 18:Y:43:ARG:N      | 18:Y:43:ARG:CZ     | 2.74                     | 0.50              |
| 1:a:5053:ILE:HA    | 1:a:5071:LEU:CD1   | 2.41                     | 0.50              |
| 1:a:5143:ILE:HD11  | 4:d:5253:TRP:CZ2   | 2.46                     | 0.50              |
| 1:a:5224:ILE:HA    | 2:b:5482:ILE:HG13  | 1.91                     | 0.50              |
| 24:a:6043:PQ9:H293 | 23:d:6039:PHO:HBA2 | 1.92                     | 0.50              |
| 2:b:5038:ALA:O     | 2:b:5042:LEU:HB2   | 2.10                     | 0.50              |
| 2:b:5074:SER:O     | 2:b:5076:SER:N     | 2.45                     | 0.50              |
| 2:b:5174:LEU:CD2   | 2:b:5312:TYR:CZ    | 2.94                     | 0.50              |
| 2:b:5483:ASP:O     | 2:b:5485:GLU:N     | 2.43                     | 0.50              |
| 22:b:6023:CLA:C4C  | 22:b:6024:CLA:HBC1 | 2.41                     | 0.50              |
| 3:c:5251:HIS:HE1   | 22:c:6030:CLA:NA   | 2.09                     | 0.50              |
| 3:c:5290:VAL:HG13  | 3:c:5427:ALA:HB2   | 1.93                     | 0.50              |
| 29:c:6056:DGD:CEB  | 29:c:6056:DGD:CIB  | 2.48                     | 0.50              |
| 10:k:5037:PHE:CB   | 25:k:6051:BCR:H401 | 2.41                     | 0.50              |
| 11:l:5032:SER:OG   | 11:l:5033:SER:N    | 2.42                     | 0.50              |
| 12:m:5018:PRO:O    | 12:m:5021:PHE:HB3  | 2.11                     | 0.50              |
| 1:A:269:ARG:HG3    | 4:D:235:PHE:HB2    | 1.94                     | 0.50              |
| 1:A:325:ASN:HB3    | 3:C:412:THR:HG21   | 1.93                     | 0.50              |
| 2:B:106:LEU:HD12   | 25:B:1048:BCR:C35  | 2.42                     | 0.50              |
| 22:B:1010:CLA:HBD  | 22:B:1010:CLA:HAA2 | 1.92                     | 0.50              |
| 3:C:142:GLU:C      | 3:C:144:SER:H      | 2.19                     | 0.50              |
| 3:C:190:ALA:O      | 3:C:191:PRO:C      | 2.54                     | 0.50              |
| 22:C:1025:CLA:O1A  | 22:C:1026:CLA:OBD  | 2.29                     | 0.50              |
| 22:C:1029:CLA:CBA  | 22:C:1029:CLA:HMA3 | 2.33                     | 0.50              |
| 4:D:37:LEU:CD1     | 4:D:125:PHE:HB2    | 2.41                     | 0.50              |
| 4:D:331:PRO:HA     | 4:D:339:PHE:HB2    | 1.92                     | 0.50              |
| 15:U:37:GLN:O      | 15:U:38:TYR:CG     | 2.64                     | 0.50              |
| 15:U:39:ARG:HH11   | 15:U:39:ARG:HG3    | 1.76                     | 0.50              |
| 20:Z:52:LEU:O      | 20:Z:55:GLY:HA3    | 2.11                     | 0.50              |
| 1:a:5053:ILE:HA    | 1:a:5071:LEU:HD13  | 1.93                     | 0.50              |
| 1:a:5296:ASN:HB3   | 3:c:5401:LEU:HD13  | 1.91                     | 0.50              |
| 1:a:5310:LYS:H     | 16:v:5028:GLU:CB   | 2.24                     | 0.50              |
| 2:b:5057:ARG:HD2   | 2:b:5311:PHE:CZ    | 2.46                     | 0.50              |
| 2:b:5099:ALA:O     | 2:b:5102:VAL:HG22  | 2.11                     | 0.50              |
| 2:b:5283:GLU:HG2   | 2:b:5286:ARG:HH12  | 1.76                     | 0.50              |
| 2:b:5297:THR:C     | 2:b:5299:GLU:N     | 2.66                     | 0.50              |
| 2:b:5354:LEU:C     | 2:b:5355:PHE:CD2   | 2.84                     | 0.50              |
| 22:b:6021:CLA:HMD2 | 22:b:6022:CLA:CBB  | 2.34                     | 0.50              |
| 3:c:5152:LYS:O     | 3:c:5154:LYS:N     | 2.45                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5184:GLY:C     | 3:c:5185:LEU:HD23  | 2.37                     | 0.50              |
| 3:c:5274:TYR:CE1   | 22:c:6029:CLA:OBD  | 2.64                     | 0.50              |
| 3:c:5438:LEU:O     | 3:c:5442:LEU:HD12  | 2.11                     | 0.50              |
| 22:c:6030:CLA:CHD  | 22:c:6030:CLA:HBC3 | 2.37                     | 0.50              |
| 22:c:6033:CLA:H2   | 22:c:6033:CLA:H72  | 1.92                     | 0.50              |
| 7:h:5035:MET:SD    | 25:h:6049:BCR:H333 | 2.51                     | 0.50              |
| 10:k:5032:PHE:CE1  | 25:k:6052:BCR:H383 | 2.43                     | 0.50              |
| 15:u:5084:VAL:CG1  | 15:u:5085:THR:N    | 2.75                     | 0.50              |
| 16:v:5038:LEU:HB3  | 16:v:5043:LYS:O    | 2.11                     | 0.50              |
| 20:z:5020:VAL:HG12 | 20:z:5021:ILE:N    | 2.26                     | 0.50              |
| 1:A:33:PHE:O       | 1:A:34:GLY:C       | 2.54                     | 0.50              |
| 22:B:1021:CLA:H112 | 28:B:1060:MGE:H131 | 1.94                     | 0.50              |
| 22:B:1024:CLA:HBC2 | 22:B:1024:CLA:CMC  | 2.41                     | 0.50              |
| 3:C:62:PHE:CZ      | 10:K:28:ILE:HB     | 2.46                     | 0.50              |
| 3:C:274:TYR:CE1    | 22:C:1029:CLA:OBD  | 2.64                     | 0.50              |
| 3:C:297:TYR:HA     | 3:C:302:TYR:CE2    | 2.46                     | 0.50              |
| 3:C:328:VAL:HG12   | 3:C:340:TYR:HB2    | 1.91                     | 0.50              |
| 4:D:261:PHE:N      | 24:D:1042:PQ9:H91  | 2.14                     | 0.50              |
| 25:D:1050:BCR:C38  | 25:D:1050:BCR:C23  | 2.59                     | 0.50              |
| 9:J:8:ILE:H        | 9:J:8:ILE:HD12     | 1.76                     | 0.50              |
| 10:K:21:LEU:O      | 10:K:24:VAL:N      | 2.44                     | 0.50              |
| 10:K:28:ILE:HD13   | 10:K:31:LEU:CD1    | 2.38                     | 0.50              |
| 12:M:11:THR:O      | 12:M:14:PHE:HB3    | 2.10                     | 0.50              |
| 13:O:105:ASP:O     | 13:O:106:GLN:HB2   | 2.12                     | 0.50              |
| 13:O:242:GLU:HG3   | 13:O:262:GLN:HG2   | 1.93                     | 0.50              |
| 1:a:5026:ASN:O     | 1:a:5028:LEU:N     | 2.44                     | 0.50              |
| 1:a:5076:ASN:HB2   | 4:d:5298:PHE:HE1   | 1.76                     | 0.50              |
| 1:a:5199:GLN:C     | 1:a:5201:GLY:N     | 2.67                     | 0.50              |
| 2:b:5327:THR:HG21  | 12:m:5004:ASN:HD22 | 1.75                     | 0.50              |
| 22:b:6010:CLA:O2D  | 22:b:6010:CLA:H2A  | 2.11                     | 0.50              |
| 22:b:6016:CLA:C17  | 22:d:6008:CLA:CMA  | 2.89                     | 0.50              |
| 28:b:6060:MGE:H6B1 | 4:d:5280:TRP:CD1   | 2.46                     | 0.50              |
| 29:b:6058:DGD:C6D  | 29:b:6058:DGD:C5E  | 2.90                     | 0.50              |
| 3:c:5297:TYR:HA    | 3:c:5302:TYR:CE2   | 2.46                     | 0.50              |
| 4:d:5273:PHE:CE2   | 28:l:6061:MGE:H5B1 | 2.47                     | 0.50              |
| 7:h:5043:LEU:CD2   | 17:x:5019:PHE:CZ   | 2.92                     | 0.50              |
| 10:k:5020:PRO:O    | 10:k:5023:ASP:HB2  | 2.11                     | 0.50              |
| 13:o:5206:GLU:O    | 13:o:5207:GLU:HB3  | 2.11                     | 0.50              |
| 15:u:5039:ARG:HH11 | 15:u:5039:ARG:HG3  | 1.76                     | 0.50              |
| 18:y:5043:ARG:NH1  | 18:y:5043:ARG:H    | 2.09                     | 0.50              |
| 18:y:5043:ARG:CZ   | 18:y:5043:ARG:N    | 2.74                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:53:ILE:HA      | 1:A:71:LEU:CD1     | 2.41                     | 0.50              |
| 1:A:116:ILE:CG2    | 1:A:117:PHE:N      | 2.74                     | 0.50              |
| 1:A:239:PHE:CZ     | 4:D:247:VAL:HA     | 2.47                     | 0.50              |
| 2:B:38:ALA:O       | 2:B:42:LEU:HB2     | 2.10                     | 0.50              |
| 2:B:153:PHE:HD1    | 2:B:157:HIS:HB3    | 1.76                     | 0.50              |
| 2:B:311:PHE:HA     | 2:B:430:PHE:CZ     | 2.46                     | 0.50              |
| 2:B:327:THR:HG21   | 12:M:4:ASN:HD22    | 1.75                     | 0.50              |
| 22:C:1031:CLA:C14  | 25:C:1054:BCR:H361 | 2.40                     | 0.50              |
| 4:D:140:PRO:O      | 4:D:141:TYR:C      | 2.53                     | 0.50              |
| 4:D:213:ILE:HG23   | 4:D:214:HIS:N      | 2.26                     | 0.50              |
| 4:D:214:HIS:O      | 4:D:217:THR:HG22   | 2.11                     | 0.50              |
| 24:D:1042:PQ9:H252 | 28:L:1061:MGE:CGB  | 2.41                     | 0.50              |
| 9:J:23:VAL:CG1     | 9:J:24:ILE:N       | 2.75                     | 0.50              |
| 12:M:20:VAL:HG11   | 12:m:5020:VAL:HG22 | 1.93                     | 0.50              |
| 15:U:58:VAL:HB     | 15:U:59:GLU:OE2    | 2.11                     | 0.50              |
| 1:a:5189:GLU:O     | 3:c:5411:ALA:HB2   | 2.11                     | 0.50              |
| 2:b:5021:ALA:HA    | 2:b:5024:LEU:HD23  | 1.94                     | 0.50              |
| 2:b:5061:PHE:HB2   | 22:b:6015:CLA:HMA1 | 1.93                     | 0.50              |
| 2:b:5080:ILE:O     | 2:b:5080:ILE:HG22  | 2.11                     | 0.50              |
| 2:b:5099:ALA:O     | 2:b:5102:VAL:CG2   | 2.59                     | 0.50              |
| 2:b:5368:VAL:HG22  | 2:b:5381:ILE:HG13  | 1.92                     | 0.50              |
| 22:b:6024:CLA:HBC2 | 22:b:6024:CLA:CMC  | 2.41                     | 0.50              |
| 3:c:5222:GLY:HA3   | 3:c:5225:VAL:CG2   | 2.41                     | 0.50              |
| 3:c:5223:TRP:CD1   | 3:c:5223:TRP:C     | 2.89                     | 0.50              |
| 4:d:5026:ARG:HH11  | 4:d:5026:ARG:HG3   | 1.76                     | 0.50              |
| 4:d:5103:ARG:HD3   | 4:d:5106:GLN:HE21  | 1.74                     | 0.50              |
| 4:d:5342:PRO:HD2   | 4:d:5345:VAL:HG21  | 1.94                     | 0.50              |
| 9:j:5023:VAL:CG1   | 9:j:5024:ILE:N     | 2.75                     | 0.50              |
| 13:o:5055:ALA:HB2  | 13:o:5163:THR:HB   | 1.94                     | 0.50              |
| 13:o:5215:ARG:HG2  | 13:o:5215:ARG:NH1  | 2.24                     | 0.50              |
| 14:t:5011:ALA:O    | 14:t:5013:ILE:N    | 2.44                     | 0.50              |
| 16:v:5160:LYS:N    | 16:v:5163:TYR:CE1  | 2.78                     | 0.50              |
| 1:A:147:TYR:O      | 1:A:150:PRO:HD2    | 2.11                     | 0.50              |
| 1:A:244:GLU:HG2    | 4:D:264:LYS:HZ2    | 1.76                     | 0.50              |
| 1:A:290:ILE:HD11   | 22:A:1003:CLA:HMD2 | 1.93                     | 0.50              |
| 2:B:28:ALA:HB2     | 2:B:107:LEU:HB2    | 1.93                     | 0.50              |
| 2:B:69:LEU:HB3     | 22:B:1014:CLA:HMA1 | 1.94                     | 0.50              |
| 2:B:90:PHE:C       | 2:B:90:PHE:HD2     | 2.18                     | 0.50              |
| 2:B:193:TYR:HE1    | 2:B:259:GLY:C      | 2.20                     | 0.50              |
| 2:B:195:PRO:O      | 2:B:196:GLY:C      | 2.53                     | 0.50              |
| 22:B:1018:CLA:HAA2 | 22:B:1018:CLA:HBD  | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:177:ALA:O      | 3:C:181:PHE:N      | 2.24                     | 0.50              |
| 3:C:222:GLY:HA3    | 3:C:225:VAL:CG2    | 2.41                     | 0.50              |
| 4:D:173:PHE:HD1    | 23:D:1039:PHO:H13  | 1.76                     | 0.50              |
| 4:D:317:LYS:HG2    | 27:D:1064:IOD:I    | 2.82                     | 0.50              |
| 13:O:62:GLN:HA     | 13:O:62:GLN:NE2    | 2.26                     | 0.50              |
| 13:O:251:MET:HE2   | 13:O:251:MET:N     | 2.26                     | 0.50              |
| 16:V:38:LEU:HB3    | 16:V:43:LYS:O      | 2.11                     | 0.50              |
| 18:Y:43:ARG:HG2    | 18:Y:44:GLY:H      | 1.73                     | 0.50              |
| 1:a:5075:ASN:HD22  | 1:a:5080:GLY:HA2   | 1.76                     | 0.50              |
| 1:a:5092:HIS:CD2   | 3:c:5219:GLY:O     | 2.64                     | 0.50              |
| 22:a:6003:CLA:HBB1 | 22:a:6006:CLA:HMD2 | 1.94                     | 0.50              |
| 2:b:5340:TRP:HE1   | 2:b:5428:GLU:HB3   | 1.76                     | 0.50              |
| 3:c:5309:ALA:C     | 3:c:5311:GLN:H     | 2.20                     | 0.50              |
| 3:c:5309:ALA:O     | 3:c:5312:ALA:N     | 2.44                     | 0.50              |
| 3:c:5327:ASN:ND2   | 3:c:5330:SER:H     | 2.09                     | 0.50              |
| 4:d:5088:SER:C     | 4:d:5090:LEU:N     | 2.69                     | 0.50              |
| 4:d:5109:GLY:O     | 4:d:5110:LEU:C     | 2.55                     | 0.50              |
| 7:h:5047:GLU:O     | 7:h:5053:LEU:N     | 2.40                     | 0.50              |
| 9:j:5038:SER:O     | 9:j:5039:SER:CB    | 2.59                     | 0.50              |
| 11:l:5005:PRO:O    | 11:l:5007:ARG:N    | 2.44                     | 0.50              |
| 11:l:5020:GLY:HA3  | 12:m:5022:LEU:CD1  | 2.42                     | 0.50              |
| 13:o:5236:GLU:C    | 13:o:5237:ILE:HG22 | 2.37                     | 0.50              |
| 15:u:5037:GLN:O    | 15:u:5038:TYR:CG   | 2.64                     | 0.50              |
| 16:v:5036:VAL:HG12 | 16:v:5150:LYS:HE3  | 1.92                     | 0.50              |
| 18:y:5039:LEU:CD2  | 20:z:5028:ALA:HB1  | 2.42                     | 0.50              |
| 18:y:5043:ARG:HG2  | 18:y:5044:GLY:H    | 1.73                     | 0.50              |
| 1:A:205:VAL:HG13   | 1:A:206:PHE:H      | 1.77                     | 0.50              |
| 2:B:60:MET:HA      | 2:B:60:MET:HE2     | 1.93                     | 0.50              |
| 22:B:1019:CLA:HBB2 | 22:B:1021:CLA:CMB  | 2.41                     | 0.50              |
| 3:C:309:ALA:O      | 3:C:312:ALA:N      | 2.44                     | 0.50              |
| 22:C:1033:CLA:H2   | 22:C:1033:CLA:H72  | 1.92                     | 0.50              |
| 22:C:1037:CLA:CB   | 22:C:1037:CLA:CHD  | 2.76                     | 0.50              |
| 25:C:1054:BCR:C23  | 25:C:1054:BCR:H402 | 2.31                     | 0.50              |
| 4:D:15:PHE:O       | 4:D:18:LEU:N       | 2.45                     | 0.50              |
| 4:D:29:PHE:CD2     | 4:D:30:VAL:N       | 2.79                     | 0.50              |
| 5:E:32:ILE:HG22    | 5:E:33:ALA:N       | 2.26                     | 0.50              |
| 12:M:18:PRO:HG2    | 12:M:19:SER:H      | 1.77                     | 0.50              |
| 13:O:154:SER:O     | 13:O:168:PHE:HA    | 2.11                     | 0.50              |
| 13:O:206:GLU:O     | 13:O:207:GLU:HB3   | 2.11                     | 0.50              |
| 14:T:8:PHE:HE1     | 27:T:1066:IOD:I    | 2.63                     | 0.50              |
| 16:V:151:ILE:HD13  | 16:V:151:ILE:N     | 2.23                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:X:13:THR:O     | 17:X:14:PRO:C      | 2.54                     | 0.50              |
| 1:a:5116:ILE:CG2  | 1:a:5117:PHE:N     | 2.74                     | 0.50              |
| 1:a:5205:VAL:HG13 | 1:a:5206:PHE:N     | 2.27                     | 0.50              |
| 1:a:5302:PHE:HB3  | 1:a:5305:SER:OG    | 2.12                     | 0.50              |
| 2:b:5052:LEU:CD2  | 2:b:5311:PHE:HD1   | 2.20                     | 0.50              |
| 2:b:5053:ASN:N    | 2:b:5054:PRO:CD    | 2.74                     | 0.50              |
| 2:b:5191:ASN:O    | 2:b:5192:PRO:C     | 2.54                     | 0.50              |
| 2:b:5310:ALA:O    | 2:b:5313:ASP:N     | 2.41                     | 0.50              |
| 2:b:5467:ILE:HD13 | 4:d:5126:MET:SD    | 2.52                     | 0.50              |
| 22:b:6011:CLA:OBD | 22:b:6013:CLA:H12  | 2.10                     | 0.50              |
| 3:c:5045:LEU:CD2  | 3:c:5141:GLU:OE1   | 2.60                     | 0.50              |
| 3:c:5142:GLU:C    | 3:c:5144:SER:H     | 2.19                     | 0.50              |
| 3:c:5315:MET:HE3  | 3:c:5315:MET:CA    | 2.37                     | 0.50              |
| 3:c:5327:ASN:C    | 3:c:5328:VAL:HG23  | 2.37                     | 0.50              |
| 3:c:5472:LEU:O    | 3:c:5473:ASP:CB    | 2.58                     | 0.50              |
| 22:c:6025:CLA:O1A | 22:c:6026:CLA:OBD  | 2.29                     | 0.50              |
| 25:d:6050:BCR:C20 | 28:d:6059:MGE:C5A  | 2.88                     | 0.50              |
| 6:f:5029:PRO:O    | 6:f:5032:PHE:HB3   | 2.11                     | 0.50              |
| 9:j:5019:MET:O    | 9:j:5023:VAL:N     | 2.45                     | 0.50              |
| 10:k:5018:PHE:O   | 10:k:5019:ASP:C    | 2.53                     | 0.50              |
| 10:k:5039:VAL:CG2 | 18:y:5036:ILE:HD11 | 2.19                     | 0.50              |
| 22:k:6034:CLA:O1A | 22:k:6034:CLA:O2D  | 2.30                     | 0.50              |
| 13:o:5221:GLY:O   | 13:o:5222:GLN:CB   | 2.59                     | 0.50              |
| 13:o:5242:GLU:HG3 | 13:o:5262:GLN:HG2  | 1.93                     | 0.50              |
| 13:o:5251:MET:HE2 | 13:o:5251:MET:N    | 2.26                     | 0.50              |
| 15:u:5016:LYS:HG2 | 15:u:5021:TYR:HD1  | 1.74                     | 0.50              |
| 1:A:33:PHE:HB2    | 1:A:129:ARG:HB2    | 1.94                     | 0.50              |
| 1:A:71:LEU:O      | 14:T:3:THR:HG21    | 2.11                     | 0.50              |
| 1:A:86:SER:C      | 1:A:88:ALA:N       | 2.68                     | 0.50              |
| 1:A:202:VAL:HG22  | 1:A:206:PHE:CD1    | 2.46                     | 0.50              |
| 1:A:214:MET:O     | 1:A:217:SER:N      | 2.43                     | 0.50              |
| 1:A:221:SER:HA    | 4:D:139:ARG:HB2    | 1.93                     | 0.50              |
| 2:B:57:ARG:HD2    | 2:B:311:PHE:CZ     | 2.46                     | 0.50              |
| 2:B:308:LYS:O     | 2:B:312:TYR:HD2    | 1.94                     | 0.50              |
| 2:B:434:THR:OG1   | 13:O:204:LYS:HD3   | 2.11                     | 0.50              |
| 22:B:1011:CLA:C1D | 22:B:1013:CLA:C4   | 2.89                     | 0.50              |
| 22:B:1023:CLA:C4C | 22:B:1024:CLA:HBC1 | 2.41                     | 0.50              |
| 3:C:309:ALA:C     | 3:C:311:GLN:H      | 2.20                     | 0.50              |
| 3:C:348:GLU:H     | 13:O:42:ALA:HB3    | 1.76                     | 0.50              |
| 3:C:438:LEU:O     | 3:C:442:LEU:HD12   | 2.11                     | 0.50              |
| 4:D:196:PHE:HB3   | 4:D:281:MET:O      | 2.12                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:D:1062:MGE:H7A2 | 14:T:21:ILE:HD11   | 1.94                     | 0.50              |
| 8:I:30:ARG:HG3     | 8:I:30:ARG:NH1     | 2.25                     | 0.50              |
| 13:O:52:ALA:HA     | 13:O:230:VAL:O     | 2.11                     | 0.50              |
| 13:O:55:ALA:HB2    | 13:O:163:THR:HB    | 1.94                     | 0.50              |
| 25:T:6048:BCR:C35  | 2:b:5106:LEU:HD12  | 2.42                     | 0.50              |
| 15:U:64:ILE:HB     | 15:U:67:LEU:CD1    | 2.38                     | 0.50              |
| 18:Y:43:ARG:CD     | 20:Z:31:GLN:NE2    | 2.75                     | 0.50              |
| 1:a:5218:LEU:CD2   | 1:a:5218:LEU:N     | 2.75                     | 0.50              |
| 1:a:5290:ILE:HD11  | 22:a:6003:CLA:HMD2 | 1.93                     | 0.50              |
| 22:a:6006:CLA:HBC1 | 4:d:5182:LEU:CD2   | 2.41                     | 0.50              |
| 2:b:5066:MET:HE3   | 2:b:5096:VAL:HB    | 1.94                     | 0.50              |
| 3:c:5063:TRP:HE1   | 22:c:6028:CLA:C3C  | 2.24                     | 0.50              |
| 3:c:5222:GLY:HA3   | 29:c:6055:DGD:O1B  | 2.12                     | 0.50              |
| 3:c:5307:PRO:HA    | 3:c:5358:PHE:CE1   | 2.47                     | 0.50              |
| 3:c:5438:LEU:CD1   | 3:c:5442:LEU:HD11  | 2.42                     | 0.50              |
| 4:d:5140:PRO:O     | 4:d:5141:TYR:C     | 2.53                     | 0.50              |
| 4:d:5152:VAL:HB    | 22:d:6004:CLA:H43  | 1.94                     | 0.50              |
| 4:d:5213:ILE:HD11  | 4:d:5253:TRP:CH2   | 2.46                     | 0.50              |
| 7:h:5019:GLY:O     | 7:h:5021:VAL:HG12  | 2.11                     | 0.50              |
| 8:i:5030:ARG:HG3   | 8:i:5030:ARG:NH1   | 2.26                     | 0.50              |
| 10:k:5028:ILE:HD13 | 10:k:5031:LEU:CD1  | 2.38                     | 0.50              |
| 13:o:5062:GLN:HA   | 13:o:5062:GLN:NE2  | 2.26                     | 0.50              |
| 18:y:5028:ILE:HG12 | 18:y:5029:GLY:N    | 2.27                     | 0.50              |
| 20:z:5025:VAL:O    | 20:z:5028:ALA:HB3  | 2.12                     | 0.50              |
| 1:A:55:ALA:H       | 1:A:70:SER:HB2     | 1.77                     | 0.50              |
| 1:A:120:LEU:HD11   | 1:A:155:PHE:CE1    | 2.46                     | 0.50              |
| 2:B:191:ASN:O      | 2:B:192:PRO:C      | 2.54                     | 0.50              |
| 2:B:456:ALA:CA     | 29:B:1058:DGD:HBV1 | 2.42                     | 0.50              |
| 3:C:222:GLY:HA3    | 29:C:1055:DGD:O1B  | 2.12                     | 0.50              |
| 3:C:307:PRO:HA     | 3:C:358:PHE:CE1    | 2.47                     | 0.50              |
| 22:C:1031:CLA:H142 | 25:C:1054:BCR:H362 | 1.91                     | 0.50              |
| 29:C:1057:DGD:HB81 | 28:D:1059:MGE:C8B  | 2.24                     | 0.50              |
| 4:D:269:PHE:O      | 4:D:272:LEU:N      | 2.38                     | 0.50              |
| 7:H:35:MET:SD      | 25:H:1049:BCR:H333 | 2.51                     | 0.50              |
| 10:K:31:LEU:O      | 10:K:34:ALA:HB3    | 2.12                     | 0.50              |
| 11:L:5:PRO:O       | 11:L:7:ARG:N       | 2.44                     | 0.50              |
| 13:O:150:ASN:HD22  | 13:O:173:ASN:CB    | 2.24                     | 0.50              |
| 13:O:200:LEU:HB3   | 13:O:203:ALA:HB2   | 1.94                     | 0.50              |
| 13:O:221:GLY:O     | 13:O:222:GLN:CB    | 2.59                     | 0.50              |
| 15:U:32:ILE:O      | 15:U:32:ILE:HG12   | 2.12                     | 0.50              |
| 16:V:36:VAL:HG12   | 16:V:150:LYS:HE3   | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:V:46:THR:O      | 16:V:47:LEU:CB     | 2.58                     | 0.50              |
| 1:a:5338:ASN:O     | 1:a:5339:PHE:CD1   | 2.65                     | 0.50              |
| 26:a:6063:LHG:H292 | 22:c:6032:CLA:C7   | 2.38                     | 0.50              |
| 2:b:5097:ALA:O     | 2:b:5099:ALA:N     | 2.45                     | 0.50              |
| 22:b:6020:CLA:O2A  | 22:b:6020:CLA:C4   | 2.59                     | 0.50              |
| 22:b:6021:CLA:H112 | 28:b:6060:MGE:H131 | 1.94                     | 0.50              |
| 3:c:5179:ALA:CA    | 3:c:5199:ILE:HD13  | 2.42                     | 0.50              |
| 3:c:5200:THR:O     | 3:c:5202:PRO:HD3   | 2.10                     | 0.50              |
| 3:c:5344:SER:OG    | 3:c:5345:PRO:HD2   | 2.12                     | 0.50              |
| 4:d:5033:SER:OG    | 4:d:5128:ARG:HG2   | 2.12                     | 0.50              |
| 4:d:5037:LEU:CD2   | 4:d:5128:ARG:HD3   | 2.27                     | 0.50              |
| 4:d:5246:MET:HE2   | 4:d:5264:LYS:HD3   | 1.93                     | 0.50              |
| 10:k:5033:PHE:O    | 10:k:5034:ALA:O    | 2.30                     | 0.50              |
| 13:o:5181:ASN:O    | 13:o:5182:PHE:CB   | 2.60                     | 0.50              |
| 15:u:5064:ILE:HB   | 15:u:5067:LEU:CD1  | 2.38                     | 0.50              |
| 16:v:5039:ASN:HD22 | 16:v:5040:SER:H    | 1.59                     | 0.50              |
| 16:v:5062:ALA:CB   | 31:v:6041:HEM:HBB1 | 2.42                     | 0.50              |
| 20:z:5012:LEU:HA   | 20:z:5050:LEU:HD13 | 1.93                     | 0.50              |
| 1:A:126:TYR:O      | 1:A:126:TYR:CD2    | 2.58                     | 0.50              |
| 1:A:189:GLU:O      | 3:C:411:ALA:HB2    | 2.11                     | 0.50              |
| 1:A:322:ASN:OD1    | 3:C:412:THR:HB     | 2.12                     | 0.50              |
| 22:A:1003:CLA:HBB1 | 22:A:1006:CLA:HMD2 | 1.94                     | 0.50              |
| 2:B:297:THR:C      | 2:B:299:GLU:N      | 2.66                     | 0.50              |
| 22:B:1021:CLA:O1A  | 22:B:1021:CLA:C2   | 2.60                     | 0.50              |
| 3:C:63:TRP:HE1     | 22:C:1028:CLA:C3C  | 2.24                     | 0.50              |
| 3:C:73:ALA:O       | 10:K:10:LYS:N      | 2.45                     | 0.50              |
| 3:C:184:GLY:C      | 3:C:185:LEU:HD23   | 2.37                     | 0.50              |
| 4:D:191:TRP:HH2    | 4:D:285:GLY:HA3    | 1.77                     | 0.50              |
| 8:I:29:ALA:O       | 8:I:30:ARG:CB      | 2.59                     | 0.50              |
| 9:J:19:MET:O       | 9:J:23:VAL:N       | 2.45                     | 0.50              |
| 11:L:20:GLY:HA3    | 12:M:22:LEU:CD1    | 2.42                     | 0.50              |
| 17:X:19:PHE:O      | 17:X:20:PHE:C      | 2.52                     | 0.50              |
| 1:a:5200:LEU:HD11  | 29:c:6057:DGD:HA92 | 1.93                     | 0.50              |
| 1:a:5224:ILE:CD1   | 1:a:5225:ARG:H     | 2.24                     | 0.50              |
| 1:a:5239:PHE:CZ    | 4:d:5247:VAL:HA    | 2.47                     | 0.50              |
| 1:a:5303:ASN:N     | 1:a:5303:ASN:ND2   | 2.60                     | 0.50              |
| 2:b:5113:TRP:C     | 2:b:5115:TRP:N     | 2.69                     | 0.50              |
| 2:b:5153:PHE:HD1   | 2:b:5157:HIS:HB3   | 1.76                     | 0.50              |
| 2:b:5325:PHE:O     | 2:b:5327:THR:HG23  | 2.12                     | 0.50              |
| 3:c:5073:ALA:O     | 10:k:5010:LYS:N    | 2.45                     | 0.50              |
| 3:c:5117:VAL:HG11  | 22:c:6027:CLA:H12  | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5171:GLY:CA    | 3:c:5174:LEU:CB    | 2.86                     | 0.50              |
| 3:c:5457:LYS:HZ2   | 4:d:5228:GLY:HA2   | 1.76                     | 0.50              |
| 22:c:6033:CLA:CMA  | 22:k:6034:CLA:HMC2 | 2.40                     | 0.50              |
| 4:d:5015:PHE:O     | 4:d:5018:LEU:N     | 2.45                     | 0.50              |
| 4:d:5122:LEU:O     | 4:d:5123:ILE:C     | 2.54                     | 0.50              |
| 4:d:5194:ASN:C     | 4:d:5194:ASN:OD1   | 2.55                     | 0.50              |
| 28:d:6062:MGE:H7A2 | 14:t:5021:ILE:HD11 | 1.94                     | 0.50              |
| 5:e:5065:LEU:HD13  | 5:e:5066:VAL:N     | 2.27                     | 0.50              |
| 12:m:5021:PHE:CE1  | 12:m:5025:LEU:HG   | 2.47                     | 0.50              |
| 13:o:5080:GLU:HB2  | 13:o:5092:VAL:HG23 | 1.93                     | 0.50              |
| 15:u:5032:ILE:O    | 15:u:5032:ILE:HG12 | 2.12                     | 0.50              |
| 16:v:5138:LEU:O    | 16:v:5141:ILE:HG22 | 2.12                     | 0.50              |
| 1:A:200:LEU:HD11   | 29:C:1057:DGD:HA92 | 1.93                     | 0.49              |
| 1:A:205:VAL:HG13   | 1:A:206:PHE:N      | 2.27                     | 0.49              |
| 1:A:224:ILE:CD1    | 1:A:225:ARG:H      | 2.24                     | 0.49              |
| 2:B:74:SER:C       | 2:B:76:SER:N       | 2.69                     | 0.49              |
| 3:C:79:LYS:HB3     | 3:C:84:GLN:HE21    | 1.75                     | 0.49              |
| 3:C:146:PHE:O      | 3:C:147:PHE:CB     | 2.59                     | 0.49              |
| 3:C:152:LYS:O      | 3:C:154:LYS:N      | 2.45                     | 0.49              |
| 3:C:175:LEU:HD23   | 3:C:176:VAL:N      | 2.27                     | 0.49              |
| 3:C:324:LEU:CD2    | 15:U:32:ILE:HD13   | 2.43                     | 0.49              |
| 22:C:1027:CLA:C15  | 25:Z:1053:BCR:C33  | 2.87                     | 0.49              |
| 4:D:147:SER:O      | 4:D:148:ALA:C      | 2.55                     | 0.49              |
| 4:D:300:SER:HA     | 12:M:2:GLU:O       | 2.12                     | 0.49              |
| 5:E:27:ILE:HG13    | 31:F:1040:HEM:HMB1 | 1.94                     | 0.49              |
| 5:E:51:ARG:O       | 5:E:53:ASP:N       | 2.45                     | 0.49              |
| 13:O:59:ASP:HB2    | 13:O:62:GLN:HB2    | 1.94                     | 0.49              |
| 13:O:181:ASN:O     | 13:O:182:PHE:CB    | 2.60                     | 0.49              |
| 15:U:84:VAL:CG1    | 15:U:85:THR:N      | 2.75                     | 0.49              |
| 16:V:35:THR:HG23   | 16:V:46:THR:HA     | 1.94                     | 0.49              |
| 1:a:5205:VAL:HG13  | 1:a:5206:PHE:H     | 1.77                     | 0.49              |
| 1:a:5325:ASN:HB3   | 3:c:5412:THR:HG21  | 1.93                     | 0.49              |
| 22:b:6011:CLA:H11  | 22:b:6011:CLA:C4A  | 2.42                     | 0.49              |
| 22:b:6013:CLA:CMB  | 22:b:6014:CLA:C1   | 2.88                     | 0.49              |
| 3:c:5071:GLU:OE1   | 3:c:5089:ILE:HB    | 2.12                     | 0.49              |
| 22:c:6028:CLA:C10  | 29:c:6056:DGD:HAS2 | 2.36                     | 0.49              |
| 4:d:5032:TRP:CE3   | 4:d:5035:ILE:HD11  | 2.47                     | 0.49              |
| 4:d:5032:TRP:HB2   | 4:d:5131:GLU:OE1   | 2.11                     | 0.49              |
| 4:d:5080:THR:HA    | 4:d:5111:TRP:CD1   | 2.47                     | 0.49              |
| 5:e:5034:GLY:HA2   | 6:f:5032:PHE:CD1   | 2.47                     | 0.49              |
| 7:h:5054:ILE:HG22  | 7:h:5055:LEU:N     | 2.27                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:k:6034:CLA:H42  | 22:k:6034:CLA:HBA1 | 1.92                     | 0.49              |
| 20:z:5052:LEU:O    | 20:z:5055:GLY:HA3  | 2.11                     | 0.49              |
| 1:A:53:ILE:HA      | 1:A:71:LEU:HD13    | 1.93                     | 0.49              |
| 1:A:227:THR:OG1    | 1:A:228:THR:N      | 2.45                     | 0.49              |
| 1:A:302:PHE:HB3    | 1:A:305:SER:OG     | 2.12                     | 0.49              |
| 2:B:308:LYS:HG2    | 2:B:312:TYR:CE2    | 2.47                     | 0.49              |
| 2:B:363:PHE:HD2    | 2:B:363:PHE:H      | 1.57                     | 0.49              |
| 22:B:1015:CLA:HBB1 | 22:B:1015:CLA:HHC  | 1.95                     | 0.49              |
| 22:B:1020:CLA:O2A  | 22:B:1020:CLA:C4   | 2.59                     | 0.49              |
| 3:C:60:ILE:HG22    | 22:K:1034:CLA:CMD  | 2.42                     | 0.49              |
| 3:C:119:LEU:HD12   | 3:C:119:LEU:C      | 2.37                     | 0.49              |
| 4:D:26:ARG:HH11    | 4:D:26:ARG:HG3     | 1.76                     | 0.49              |
| 4:D:32:TRP:CE3     | 4:D:35:ILE:HD11    | 2.47                     | 0.49              |
| 4:D:33:SER:OG      | 4:D:128:ARG:HG3    | 2.11                     | 0.49              |
| 4:D:48:TRP:CZ2     | 4:D:52:THR:HG21    | 2.47                     | 0.49              |
| 4:D:88:SER:C       | 4:D:90:LEU:N       | 2.69                     | 0.49              |
| 4:D:103:ARG:HD3    | 4:D:106:GLN:HE21   | 1.74                     | 0.49              |
| 4:D:246:MET:CE     | 4:D:264:LYS:HD3    | 2.43                     | 0.49              |
| 4:D:261:PHE:HB2    | 24:D:1042:PQ9:C10  | 2.42                     | 0.49              |
| 5:E:34:GLY:HA2     | 6:F:32:PHE:CD1     | 2.46                     | 0.49              |
| 7:H:38:PHE:CZ      | 7:H:42:LEU:HD21    | 2.47                     | 0.49              |
| 11:L:30:LEU:C      | 11:L:30:LEU:CD2    | 2.83                     | 0.49              |
| 13:O:111:LEU:HD11  | 13:O:119:LEU:HB3   | 1.94                     | 0.49              |
| 16:V:67:HIS:CE1    | 16:V:80:LEU:HD11   | 2.47                     | 0.49              |
| 16:V:96:GLU:O      | 16:V:97:GLY:C      | 2.55                     | 0.49              |
| 18:Y:43:ARG:CG     | 18:Y:44:GLY:N      | 2.66                     | 0.49              |
| 2:b:5074:SER:C     | 2:b:5076:SER:N     | 2.69                     | 0.49              |
| 2:b:5308:LYS:HG2   | 2:b:5312:TYR:CE2   | 2.47                     | 0.49              |
| 2:b:5401:PHE:CZ    | 2:b:5406:LEU:HD23  | 2.47                     | 0.49              |
| 3:c:5202:PRO:HB3   | 3:c:5235:GLY:CA    | 2.40                     | 0.49              |
| 3:c:5265:ILE:CG2   | 3:c:5270:ALA:CB    | 2.90                     | 0.49              |
| 22:c:6029:CLA:CBA  | 22:c:6029:CLA:HMA3 | 2.33                     | 0.49              |
| 22:c:6032:CLA:H161 | 29:c:6056:DGD:HBH1 | 1.94                     | 0.49              |
| 4:d:5193:LEU:HA    | 4:d:5198:MET:CE    | 2.43                     | 0.49              |
| 4:d:5251:ARG:HH22  | 4:d:5255:GLN:NE2   | 2.10                     | 0.49              |
| 4:d:5302:GLU:O     | 4:d:5305:ALA:HB3   | 2.13                     | 0.49              |
| 5:e:5051:ARG:O     | 5:e:5053:ASP:N     | 2.46                     | 0.49              |
| 10:k:5021:LEU:O    | 10:k:5024:VAL:N    | 2.44                     | 0.49              |
| 11:l:5030:LEU:C    | 11:l:5030:LEU:CD2  | 2.83                     | 0.49              |
| 13:o:5116:ASP:OD2  | 13:o:5157:PRO:HB3  | 2.12                     | 0.49              |
| 13:o:5128:ASP:OD1  | 13:o:5149:LYS:CG   | 2.61                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:v:5090:PRO:O    | 16:v:5091:PRO:C    | 2.55                     | 0.49              |
| 18:y:5030:ILE:O    | 18:y:5030:ILE:HD13 | 2.12                     | 0.49              |
| 1:A:321:ILE:CD1    | 4:D:176:ALA:HB1    | 2.17                     | 0.49              |
| 25:A:1044:BCR:C8   | 25:A:1044:BCR:C33  | 2.86                     | 0.49              |
| 2:B:25:MET:HE2     | 25:B:1045:BCR:H403 | 1.94                     | 0.49              |
| 2:B:325:PHE:O      | 2:B:327:THR:HG23   | 2.12                     | 0.49              |
| 22:B:1021:CLA:O1A  | 22:B:1021:CLA:O2D  | 2.30                     | 0.49              |
| 29:B:1058:DGD:C6D  | 29:B:1058:DGD:C5E  | 2.90                     | 0.49              |
| 3:C:39:ASN:CB      | 22:C:1032:CLA:HBA1 | 2.35                     | 0.49              |
| 3:C:62:PHE:HB2     | 3:C:122:SER:CB     | 2.42                     | 0.49              |
| 3:C:71:GLU:OE1     | 3:C:89:ILE:HB      | 2.12                     | 0.49              |
| 3:C:344:SER:OG     | 3:C:345:PRO:HD2    | 2.12                     | 0.49              |
| 22:C:1027:CLA:H141 | 25:Z:1053:BCR:H333 | 1.94                     | 0.49              |
| 4:D:109:GLY:O      | 4:D:110:LEU:C      | 2.55                     | 0.49              |
| 4:D:195:PRO:HA     | 4:D:198:MET:SD     | 2.53                     | 0.49              |
| 4:D:249:ALA:O      | 4:D:252:PHE:HB3    | 2.11                     | 0.49              |
| 4:D:265:ARG:CD     | 4:D:265:ARG:C      | 2.85                     | 0.49              |
| 5:E:65:LEU:HD13    | 5:E:66:VAL:N       | 2.27                     | 0.49              |
| 6:F:29:PRO:O       | 6:F:32:PHE:HB3     | 2.11                     | 0.49              |
| 7:H:19:GLY:O       | 7:H:21:VAL:HG12    | 2.11                     | 0.49              |
| 7:H:34:PHE:CD2     | 22:H:1017:CLA:HAC1 | 2.47                     | 0.49              |
| 7:H:54:ILE:HG22    | 7:H:55:LEU:N       | 2.27                     | 0.49              |
| 9:J:38:SER:O       | 9:J:39:SER:CB      | 2.59                     | 0.49              |
| 13:O:223:ILE:HG22  | 13:O:243:SER:CB    | 2.36                     | 0.49              |
| 20:Z:25:VAL:O      | 20:Z:28:ALA:HB3    | 2.12                     | 0.49              |
| 2:b:5149:LEU:CD2   | 22:b:6011:CLA:HBC1 | 2.42                     | 0.49              |
| 2:b:5174:LEU:CD2   | 2:b:5312:TYR:CE1   | 2.95                     | 0.49              |
| 2:b:5308:LYS:O     | 2:b:5312:TYR:HD2   | 1.94                     | 0.49              |
| 22:b:6021:CLA:HAA2 | 22:b:6021:CLA:HBD  | 1.94                     | 0.49              |
| 3:c:5175:LEU:HD23  | 3:c:5176:VAL:N     | 2.27                     | 0.49              |
| 3:c:5190:ALA:O     | 3:c:5191:PRO:C     | 2.54                     | 0.49              |
| 3:c:5206:PRO:HG2   | 3:c:5207:ARG:NH1   | 2.26                     | 0.49              |
| 3:c:5274:TYR:CE1   | 22:c:6029:CLA:O1D  | 2.62                     | 0.49              |
| 3:c:5324:LEU:CD2   | 15:u:5032:ILE:HD13 | 2.43                     | 0.49              |
| 3:c:5400:PRO:O     | 3:c:5401:LEU:HD22  | 2.12                     | 0.49              |
| 3:c:5438:LEU:HD13  | 3:c:5442:LEU:HD11  | 1.94                     | 0.49              |
| 22:c:6031:CLA:C14  | 25:c:6054:BCR:H361 | 2.40                     | 0.49              |
| 4:d:5024:ARG:HA    | 4:d:5024:ARG:HE    | 1.77                     | 0.49              |
| 4:d:5091:LEU:HD23  | 4:d:5093:TRP:CE2   | 2.47                     | 0.49              |
| 4:d:5120:PHE:O     | 4:d:5121:GLY:C     | 2.55                     | 0.49              |
| 4:d:5126:MET:CE    | 4:d:5146:PHE:HB3   | 2.40                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5195:PRO:HA    | 4:d:5198:MET:SD    | 2.53                     | 0.49              |
| 5:e:5032:ILE:HG22  | 5:e:5033:ALA:N     | 2.26                     | 0.49              |
| 15:u:5025:ILE:HD11 | 15:u:5034:ALA:O    | 2.13                     | 0.49              |
| 1:A:112:TYR:O      | 1:A:113:GLN:C      | 2.55                     | 0.49              |
| 1:A:135:TYR:CD1    | 3:C:449:ARG:HG3    | 2.48                     | 0.49              |
| 1:A:215:HIS:O      | 1:A:219:VAL:HG23   | 2.11                     | 0.49              |
| 1:A:218:LEU:N      | 1:A:218:LEU:CD2    | 2.75                     | 0.49              |
| 1:A:279:ARG:CZ     | 1:A:283:VAL:HG21   | 2.42                     | 0.49              |
| 22:A:1006:CLA:H143 | 24:A:1043:PQ9:H443 | 1.94                     | 0.49              |
| 2:B:16:PRO:O       | 2:B:20:ILE:HG12    | 2.12                     | 0.49              |
| 2:B:53:ASN:N       | 2:B:54:PRO:CD      | 2.74                     | 0.49              |
| 22:B:1021:CLA:HAA2 | 22:B:1021:CLA:HBD  | 1.94                     | 0.49              |
| 3:C:45:LEU:CD2     | 3:C:141:GLU:OE1    | 2.60                     | 0.49              |
| 22:C:1027:CLA:H141 | 25:Z:1053:BCR:C33  | 2.42                     | 0.49              |
| 22:C:1033:CLA:CMA  | 22:K:1034:CLA:HMC2 | 2.40                     | 0.49              |
| 10:K:24:VAL:C      | 10:K:26:PRO:HD2    | 2.37                     | 0.49              |
| 10:K:37:PHE:HB2    | 25:K:1051:BCR:H401 | 1.94                     | 0.49              |
| 11:L:9:PRO:HB2     | 12:m:5034:LYS:HE2  | 1.93                     | 0.49              |
| 18:Y:28:ILE:HG12   | 18:Y:29:GLY:N      | 2.27                     | 0.49              |
| 1:a:5071:LEU:HD12  | 1:a:5071:LEU:H     | 1.78                     | 0.49              |
| 1:a:5258:LEU:O     | 1:a:5259:ILE:HG13  | 2.12                     | 0.49              |
| 2:b:5271:THR:HG23  | 2:b:5274:GLN:CB    | 2.42                     | 0.49              |
| 2:b:5311:PHE:HA    | 2:b:5430:PHE:CZ    | 2.46                     | 0.49              |
| 22:b:6014:CLA:HBA1 | 22:b:6014:CLA:CBF  | 2.43                     | 0.49              |
| 3:c:5048:LYS:HD2   | 22:c:6035:CLA:CED  | 2.33                     | 0.49              |
| 3:c:5362:ARG:HH22  | 13:o:5034:ASP:CG   | 2.20                     | 0.49              |
| 22:c:6027:CLA:H141 | 25:z:6053:BCR:C33  | 2.42                     | 0.49              |
| 22:c:6035:CLA:CMB  | 25:k:6052:BCR:C27  | 2.90                     | 0.49              |
| 4:d:5196:PHE:HB3   | 4:d:5281:MET:O     | 2.12                     | 0.49              |
| 9:j:5025:VAL:HA    | 9:j:5028:PHE:CD2   | 2.43                     | 0.49              |
| 2:B:168:VAL:CG1    | 2:B:169:SER:N      | 2.76                     | 0.49              |
| 2:B:308:LYS:HG2    | 2:B:312:TYR:HE2    | 1.78                     | 0.49              |
| 22:B:1011:CLA:H11  | 22:B:1011:CLA:C4A  | 2.42                     | 0.49              |
| 22:B:1019:CLA:CBB  | 22:B:1021:CLA:HMB3 | 2.43                     | 0.49              |
| 3:C:179:ALA:CA     | 3:C:199:ILE:HD13   | 2.42                     | 0.49              |
| 3:C:250:TRP:CD1    | 3:C:250:TRP:C      | 2.90                     | 0.49              |
| 3:C:265:ILE:CG2    | 3:C:270:ALA:CB     | 2.90                     | 0.49              |
| 22:C:1030:CLA:CHD  | 22:C:1030:CLA:HBC3 | 2.37                     | 0.49              |
| 5:E:31:PHE:O       | 6:F:35:GLY:HA3     | 2.13                     | 0.49              |
| 6:F:19:ARG:HH22    | 31:F:1040:HEM:CAC  | 2.17                     | 0.49              |
| 1:a:5071:LEU:O     | 14:t:5003:THR:HG21 | 2.11                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5161:TYR:CE2   | 1:a:5186:PHE:HE2   | 2.30                     | 0.49              |
| 2:b:5018:ARG:HH11  | 11:l:5004:ASN:HD22 | 1.60                     | 0.49              |
| 2:b:5028:ALA:HB2   | 2:b:5107:LEU:HB2   | 1.92                     | 0.49              |
| 2:b:5090:PHE:C     | 2:b:5090:PHE:HD2   | 2.18                     | 0.49              |
| 2:b:5109:LEU:O     | 2:b:5110:ALA:C     | 2.54                     | 0.49              |
| 2:b:5193:TYR:HE1   | 2:b:5259:GLY:C     | 2.20                     | 0.49              |
| 2:b:5278:SER:HB3   | 2:b:5281:GLN:CG    | 2.28                     | 0.49              |
| 2:b:5475:PHE:C     | 2:b:5477:ASP:N     | 2.69                     | 0.49              |
| 3:c:5062:PHE:HB2   | 3:c:5122:SER:CB    | 2.42                     | 0.49              |
| 3:c:5146:PHE:O     | 3:c:5147:PHE:CB    | 2.59                     | 0.49              |
| 3:c:5443:TRP:HD1   | 22:c:6032:CLA:CMD  | 2.25                     | 0.49              |
| 22:c:6028:CLA:H18  | 29:c:6056:DGD:HA51 | 1.94                     | 0.49              |
| 4:d:5073:PHE:HB2   | 28:d:6059:MGE:H2B2 | 1.95                     | 0.49              |
| 4:d:5173:PHE:HD1   | 23:d:6039:PHO:H13  | 1.76                     | 0.49              |
| 4:d:5265:ARG:CD    | 4:d:5265:ARG:C     | 2.86                     | 0.49              |
| 22:d:6004:CLA:HBC3 | 22:d:6004:CLA:HHD  | 1.95                     | 0.49              |
| 9:j:5010:LEU:O     | 9:j:5013:VAL:CG1   | 2.60                     | 0.49              |
| 13:o:5052:ALA:HA   | 13:o:5230:VAL:O    | 2.11                     | 0.49              |
| 13:o:5148:VAL:HA   | 13:o:5172:PHE:CE2  | 2.47                     | 0.49              |
| 16:v:5035:THR:HG23 | 16:v:5046:THR:HA   | 1.94                     | 0.49              |
| 1:A:71:LEU:HD12    | 1:A:71:LEU:H       | 1.77                     | 0.49              |
| 1:A:113:GLN:HA     | 1:A:116:ILE:HG22   | 1.95                     | 0.49              |
| 1:A:141:PRO:C      | 1:A:143:ILE:N      | 2.71                     | 0.49              |
| 1:A:219:VAL:HB     | 4:D:268:HIS:HB3    | 1.95                     | 0.49              |
| 1:A:224:ILE:HB     | 1:A:245:THR:O      | 2.12                     | 0.49              |
| 1:A:265:PHE:CE1    | 24:A:1043:PQ9:H143 | 2.48                     | 0.49              |
| 2:B:97:ALA:O       | 2:B:99:ALA:N       | 2.45                     | 0.49              |
| 2:B:215:PHE:C      | 2:B:215:PHE:HD2    | 2.20                     | 0.49              |
| 3:C:209:ILE:HD12   | 3:C:239:TRP:CD1    | 2.48                     | 0.49              |
| 3:C:270:ALA:O      | 3:C:273:SER:HB3    | 2.12                     | 0.49              |
| 3:C:296:VAL:HG23   | 3:C:297:TYR:HD1    | 1.70                     | 0.49              |
| 3:C:327:ASN:C      | 3:C:328:VAL:HG23   | 2.37                     | 0.49              |
| 3:C:342:MET:HG2    | 3:C:343:ARG:H      | 1.77                     | 0.49              |
| 3:C:400:PRO:O      | 3:C:401:LEU:HD22   | 2.12                     | 0.49              |
| 4:D:32:TRP:HB2     | 4:D:131:GLU:OE1    | 2.11                     | 0.49              |
| 4:D:61:HIS:CE1     | 4:D:80:THR:CG2     | 2.96                     | 0.49              |
| 4:D:73:PHE:HB2     | 28:D:1059:MGE:H2B2 | 1.95                     | 0.49              |
| 4:D:152:VAL:HB     | 22:D:1004:CLA:H43  | 1.94                     | 0.49              |
| 24:D:1042:PQ9:H42  | 24:D:1042:PQ9:H391 | 0.62                     | 0.49              |
| 7:H:34:PHE:CE2     | 22:H:1017:CLA:HAC1 | 2.48                     | 0.49              |
| 7:H:40:VAL:O       | 7:H:44:ILE:HG12    | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:K:18:PHE:O      | 10:K:19:ASP:C      | 2.53                     | 0.49              |
| 12:M:32:GLN:NE2    | 12:m:5034:LYS:HD2  | 2.27                     | 0.49              |
| 13:O:116:ASP:OD2   | 13:O:157:PRO:HB3   | 2.12                     | 0.49              |
| 13:O:239:GLY:O     | 13:O:265:PHE:N     | 2.44                     | 0.49              |
| 16:V:96:GLU:O      | 16:V:99:VAL:N      | 2.39                     | 0.49              |
| 16:V:154:ASP:C     | 16:V:156:TRP:N     | 2.70                     | 0.49              |
| 17:X:16:LEU:C      | 17:X:16:LEU:HD23   | 2.38                     | 0.49              |
| 18:Y:43:ARG:N      | 18:Y:43:ARG:NE     | 2.61                     | 0.49              |
| 1:a:5121:LEU:C     | 1:a:5123:ALA:N     | 2.70                     | 0.49              |
| 1:a:5135:TYR:CD1   | 3:c:5449:ARG:HG3   | 2.48                     | 0.49              |
| 1:a:5303:ASN:OD1   | 1:a:5322:ASN:ND2   | 2.46                     | 0.49              |
| 2:b:5338:GLN:O     | 2:b:5339:ALA:HB2   | 2.13                     | 0.49              |
| 2:b:5451:PHE:C     | 2:b:5451:PHE:CD2   | 2.90                     | 0.49              |
| 22:b:6011:CLA:H202 | 7:h:5038:PHE:HE2   | 1.78                     | 0.49              |
| 3:c:5171:GLY:C     | 22:c:6025:CLA:HBC3 | 2.35                     | 0.49              |
| 3:c:5209:ILE:HD12  | 3:c:5239:TRP:CD1   | 2.48                     | 0.49              |
| 4:d:5249:ALA:O     | 4:d:5252:PHE:HB3   | 2.12                     | 0.49              |
| 4:d:5300:SER:HA    | 12:m:5002:GLU:O    | 2.12                     | 0.49              |
| 22:h:6017:CLA:HBB1 | 25:h:6049:BCR:C32  | 2.42                     | 0.49              |
| 25:h:6049:BCR:HC8  | 25:h:6049:BCR:C32  | 2.40                     | 0.49              |
| 8:i:5024:LEU:C     | 8:i:5026:GLY:N     | 2.70                     | 0.49              |
| 10:k:5024:VAL:C    | 10:k:5026:PRO:HD2  | 2.37                     | 0.49              |
| 13:o:5163:THR:O    | 13:o:5165:SER:N    | 2.46                     | 0.49              |
| 16:v:5109:ASP:OD1  | 16:v:5111:GLU:HG3  | 2.12                     | 0.49              |
| 16:v:5154:ASP:C    | 16:v:5156:TRP:H    | 2.21                     | 0.49              |
| 17:x:5013:THR:O    | 17:x:5014:PRO:C    | 2.54                     | 0.49              |
| 1:A:121:LEU:C      | 1:A:123:ALA:N      | 2.70                     | 0.49              |
| 1:A:142:TRP:HE1    | 4:D:219:GLU:CB     | 2.25                     | 0.49              |
| 1:A:161:TYR:CE2    | 1:A:186:PHE:HE2    | 2.30                     | 0.49              |
| 1:A:187:GLN:NE2    | 1:A:193:LEU:HB2    | 2.27                     | 0.49              |
| 1:A:225:ARG:CB     | 2:B:484:PRO:HD3    | 2.43                     | 0.49              |
| 23:A:1038:PHO:O1D  | 23:A:1038:PHO:C2A  | 2.57                     | 0.49              |
| 2:B:6:TYR:CD2      | 2:B:6:TYR:N        | 2.76                     | 0.49              |
| 2:B:69:LEU:CD1     | 22:B:1011:CLA:OBD  | 2.59                     | 0.49              |
| 2:B:115:TRP:HB3    | 27:B:1067:IOD:I    | 2.82                     | 0.49              |
| 2:B:463:PHE:CE1    | 22:B:1016:CLA:CBB  | 2.89                     | 0.49              |
| 22:B:1016:CLA:H162 | 22:D:1008:CLA:HMA3 | 1.70                     | 0.49              |
| 22:B:1016:CLA:C17  | 22:D:1008:CLA:CMA  | 2.89                     | 0.49              |
| 3:C:29:GLU:HA      | 3:C:41:ARG:HH11    | 1.74                     | 0.49              |
| 3:C:72:LEU:CD1     | 3:C:112:PHE:HB2    | 2.43                     | 0.49              |
| 3:C:105:VAL:O      | 3:C:105:VAL:CG2    | 2.61                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:438:LEU:CD1    | 3:C:442:LEU:HD11   | 2.42                     | 0.49              |
| 4:D:101:PHE:O      | 4:D:101:PHE:CG     | 2.65                     | 0.49              |
| 4:D:273:PHE:CE2    | 28:L:1061:MGE:H5B1 | 2.47                     | 0.49              |
| 4:D:286:VAL:O      | 4:D:287:VAL:C      | 2.56                     | 0.49              |
| 7:H:18:TYR:CD2     | 7:H:18:TYR:C       | 2.90                     | 0.49              |
| 9:J:10:LEU:O       | 9:J:13:VAL:CG1     | 2.60                     | 0.49              |
| 13:O:128:ASP:OD1   | 13:O:149:LYS:CG    | 2.61                     | 0.49              |
| 16:V:38:LEU:HA     | 16:V:45:ILE:HD11   | 1.94                     | 0.49              |
| 16:V:64:ALA:O      | 16:V:68:VAL:N      | 2.46                     | 0.49              |
| 16:V:114:ILE:CD1   | 31:V:1041:HEM:HBD2 | 2.43                     | 0.49              |
| 16:V:138:LEU:O     | 16:V:141:ILE:HG22  | 2.12                     | 0.49              |
| 16:V:154:ASP:C     | 16:V:156:TRP:H     | 2.21                     | 0.49              |
| 1:a:5141:PRO:C     | 1:a:5143:ILE:N     | 2.70                     | 0.49              |
| 1:a:5221:SER:HA    | 4:d:5139:ARG:HB2   | 1.93                     | 0.49              |
| 2:b:5069:LEU:HB3   | 22:b:6014:CLA:HMA1 | 1.94                     | 0.49              |
| 2:b:5121:GLU:CG    | 7:h:5012:ARG:HD3   | 2.40                     | 0.49              |
| 2:b:5460:LEU:HD12  | 4:d:5159:ILE:CD1   | 2.42                     | 0.49              |
| 22:b:6015:CLA:HBB1 | 22:b:6015:CLA:HHC  | 1.94                     | 0.49              |
| 3:c:5449:ARG:HB2   | 22:c:6029:CLA:CED  | 2.43                     | 0.49              |
| 22:c:6035:CLA:HBB2 | 22:k:6034:CLA:CMA  | 2.31                     | 0.49              |
| 4:d:5053:THR:CG2   | 4:d:5067:TYR:HD2   | 2.26                     | 0.49              |
| 4:d:5087:HIS:C     | 4:d:5167:TRP:HE1   | 2.20                     | 0.49              |
| 4:d:5246:MET:CE    | 4:d:5264:LYS:HD3   | 2.43                     | 0.49              |
| 5:e:5013:ILE:CG1   | 5:e:5019:TYR:HB2   | 2.43                     | 0.49              |
| 10:k:5037:PHE:O    | 10:k:5038:VAL:C    | 2.55                     | 0.49              |
| 17:x:5016:LEU:HD23 | 17:x:5016:LEU:C    | 2.38                     | 0.49              |
| 18:y:5042:ARG:HB3  | 18:y:5043:ARG:NE   | 2.28                     | 0.49              |
| 18:y:5043:ARG:CD   | 20:z:5031:GLN:NE2  | 2.75                     | 0.49              |
| 20:z:5053:VAL:HG12 | 20:z:5057:LEU:HD12 | 1.95                     | 0.49              |
| 2:B:80:ILE:O       | 2:B:80:ILE:HG22    | 2.11                     | 0.49              |
| 2:B:120:LEU:HD23   | 2:B:120:LEU:N      | 2.28                     | 0.49              |
| 2:B:201:HIS:HD2    | 2:B:202:HIS:CD2    | 2.30                     | 0.49              |
| 2:B:401:PHE:CZ     | 2:B:406:LEU:HD23   | 2.47                     | 0.49              |
| 2:B:460:LEU:HD12   | 4:D:159:ILE:CD1    | 2.42                     | 0.49              |
| 3:C:39:ASN:HB3     | 22:C:1033:CLA:CBB  | 2.43                     | 0.49              |
| 3:C:438:LEU:HD13   | 3:C:442:LEU:HD11   | 1.94                     | 0.49              |
| 3:C:443:TRP:HD1    | 22:C:1032:CLA:CMD  | 2.25                     | 0.49              |
| 4:D:80:THR:HA      | 4:D:111:TRP:CD1    | 2.47                     | 0.49              |
| 4:D:88:SER:CA      | 7:H:50:ASN:HD21    | 2.03                     | 0.49              |
| 4:D:91:LEU:HD23    | 4:D:93:TRP:CE2     | 2.47                     | 0.49              |
| 22:D:1004:CLA:HBC3 | 22:D:1004:CLA:HHD  | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F:28:VAL:HB      | 6:F:29:PRO:CD      | 2.38                     | 0.49              |
| 6:F:32:PHE:CD1     | 6:F:32:PHE:C       | 2.87                     | 0.49              |
| 7:H:12:ARG:NH1     | 7:H:12:ARG:O       | 2.45                     | 0.49              |
| 9:J:39:SER:O       | 9:J:40:LEU:HD23    | 2.13                     | 0.49              |
| 14:T:24:ARG:HD2    | 14:T:24:ARG:C      | 2.38                     | 0.49              |
| 16:V:62:ALA:CB     | 31:V:1041:HEM:HBB1 | 2.42                     | 0.49              |
| 18:Y:30:ILE:O      | 18:Y:30:ILE:HD13   | 2.12                     | 0.49              |
| 18:Y:43:ARG:NH1    | 18:Y:43:ARG:H      | 2.09                     | 0.49              |
| 1:a:5048:PHE:O     | 1:a:5050:ILE:N     | 2.46                     | 0.49              |
| 1:a:5142:TRP:CH2   | 26:a:6063:LHG:HC5  | 2.47                     | 0.49              |
| 1:a:5142:TRP:HE1   | 4:d:5219:GLU:CB    | 2.25                     | 0.49              |
| 1:a:5195:HIS:CE1   | 1:a:5197:PHE:HB2   | 2.48                     | 0.49              |
| 1:a:5216:GLY:HA3   | 4:d:5268:HIS:O     | 2.12                     | 0.49              |
| 1:a:5223:LEU:CD2   | 4:d:5265:ARG:HG2   | 2.35                     | 0.49              |
| 1:a:5265:PHE:CE1   | 24:a:6043:PQ9:H143 | 2.48                     | 0.49              |
| 1:a:5335:ASN:OD1   | 1:a:5335:ASN:N     | 2.43                     | 0.49              |
| 2:b:5016:PRO:O     | 2:b:5020:ILE:HG12  | 2.12                     | 0.49              |
| 2:b:5025:MET:HE2   | 25:b:6045:BCR:H403 | 1.94                     | 0.49              |
| 2:b:5069:LEU:CD1   | 22:b:6011:CLA:OBD  | 2.59                     | 0.49              |
| 2:b:5257:TRP:CD2   | 4:d:5291:LEU:HD22  | 2.48                     | 0.49              |
| 22:b:6018:CLA:HAA2 | 22:b:6018:CLA:HBD  | 1.94                     | 0.49              |
| 22:b:6021:CLA:HMA2 | 22:b:6021:CLA:O2A  | 2.13                     | 0.49              |
| 3:c:5414:ILE:CG2   | 3:c:5415:ASN:N     | 2.76                     | 0.49              |
| 3:c:5440:GLY:O     | 3:c:5441:HIS:C     | 2.56                     | 0.49              |
| 3:c:5459:ILE:N     | 4:d:5224:GLN:H     | 2.08                     | 0.49              |
| 4:d:5061:HIS:CE1   | 4:d:5080:THR:CG2   | 2.96                     | 0.49              |
| 4:d:5088:SER:HB2   | 5:e:5069:ARG:NH2   | 2.28                     | 0.49              |
| 6:f:5019:ARG:NH2   | 6:f:5020:TRP:CD1   | 2.81                     | 0.49              |
| 7:h:5007:LEU:HA    | 7:h:5010:ILE:HD12  | 1.94                     | 0.49              |
| 7:h:5012:ARG:NH1   | 7:h:5012:ARG:O     | 2.45                     | 0.49              |
| 9:j:5039:SER:O     | 9:j:5040:LEU:HD23  | 2.13                     | 0.49              |
| 13:o:5105:ASP:O    | 13:o:5106:GLN:HB2  | 2.12                     | 0.49              |
| 16:v:5067:HIS:CE1  | 16:v:5080:LEU:HD11 | 2.47                     | 0.49              |
| 1:A:257:ARG:O      | 1:A:259:ILE:N      | 2.46                     | 0.49              |
| 2:B:52:LEU:CD2     | 2:B:311:PHE:HD1    | 2.20                     | 0.49              |
| 2:B:338:GLN:O      | 2:B:339:ALA:HB2    | 2.13                     | 0.49              |
| 2:B:418:LYS:O      | 2:B:421:ALA:N      | 2.43                     | 0.49              |
| 2:B:457:VAL:CG1    | 4:D:284:ILE:HG23   | 2.43                     | 0.49              |
| 22:B:1014:CLA:HBA1 | 22:B:1014:CLA:CBD  | 2.43                     | 0.49              |
| 22:B:1015:CLA:HAC2 | 25:t:1046:BCR:H282 | 1.88                     | 0.49              |
| 22:B:1016:CLA:H51  | 22:H:1017:CLA:H91  | 1.76                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1021:CLA:O2A  | 22:B:1021:CLA:HMA2 | 2.13                     | 0.49              |
| 3:C:88:LEU:CD1     | 22:C:1027:CLA:HBC2 | 2.42                     | 0.49              |
| 4:D:148:ALA:CB     | 4:D:149:PRO:HD3    | 2.29                     | 0.49              |
| 4:D:193:LEU:HA     | 4:D:198:MET:CE     | 2.43                     | 0.49              |
| 22:K:1034:CLA:O1A  | 22:K:1034:CLA:O2D  | 2.30                     | 0.49              |
| 12:M:20:VAL:HG11   | 12:m:5020:VAL:CG2  | 2.43                     | 0.49              |
| 12:M:21:PHE:CE1    | 12:M:25:LEU:HG     | 2.47                     | 0.49              |
| 14:T:19:PHE:N      | 14:T:19:PHE:HD2    | 2.10                     | 0.49              |
| 16:V:95:ILE:HA     | 16:V:146:LEU:HD11  | 1.95                     | 0.49              |
| 16:V:103:LYS:CE    | 16:V:138:LEU:HD12  | 2.43                     | 0.49              |
| 1:a:5118:HIS:O     | 1:a:5121:LEU:HB3   | 2.13                     | 0.49              |
| 1:a:5227:THR:OG1   | 1:a:5228:THR:N     | 2.45                     | 0.49              |
| 23:a:6038:PHO:C4C  | 4:d:5209:LEU:HG    | 2.43                     | 0.49              |
| 2:b:5201:HIS:HD2   | 2:b:5202:HIS:CD2   | 2.30                     | 0.49              |
| 2:b:5457:VAL:CG1   | 4:d:5284:ILE:HG23  | 2.43                     | 0.49              |
| 2:b:5486:LEU:O     | 2:b:5488:PRO:HD3   | 2.12                     | 0.49              |
| 22:b:6010:CLA:O2D  | 22:b:6010:CLA:O1A  | 2.30                     | 0.49              |
| 22:b:6020:CLA:H111 | 22:b:6020:CLA:H162 | 1.95                     | 0.49              |
| 22:b:6023:CLA:H93  | 22:b:6024:CLA:H152 | 1.95                     | 0.49              |
| 3:c:5105:VAL:O     | 3:c:5105:VAL:CG2   | 2.61                     | 0.49              |
| 3:c:5315:MET:HE2   | 3:c:5319:ILE:HG13  | 1.95                     | 0.49              |
| 3:c:5437:PHE:O     | 3:c:5440:GLY:N     | 2.46                     | 0.49              |
| 22:c:6025:CLA:C3A  | 22:c:6025:CLA:CGA  | 2.90                     | 0.49              |
| 5:e:5007:GLU:OE2   | 6:f:5019:ARG:HB2   | 2.13                     | 0.49              |
| 7:h:5034:PHE:CD2   | 22:h:6017:CLA:HAC1 | 2.47                     | 0.49              |
| 11:l:5005:PRO:HG2  | 11:l:5006:ASN:H    | 1.77                     | 0.49              |
| 13:o:5111:LEU:HD11 | 13:o:5119:LEU:HB3  | 1.94                     | 0.49              |
| 13:o:5162:ILE:CD1  | 13:o:5269:ILE:HD12 | 2.43                     | 0.49              |
| 15:u:5085:THR:O    | 15:u:5086:GLU:C    | 2.56                     | 0.49              |
| 16:v:5160:LYS:O    | 16:v:5163:TYR:HB2  | 2.13                     | 0.49              |
| 20:z:5015:LEU:HD11 | 20:z:5046:LEU:HG   | 1.95                     | 0.49              |
| 1:A:48:PHE:O       | 1:A:50:ILE:N       | 2.46                     | 0.49              |
| 1:A:172:MET:HE2    | 1:A:179:THR:HA     | 1.95                     | 0.49              |
| 1:A:290:ILE:HA     | 1:A:290:ILE:HD12   | 1.65                     | 0.49              |
| 2:B:30:VAL:HG13    | 22:B:1013:CLA:CMD  | 2.43                     | 0.49              |
| 2:B:95:GLY:O       | 2:B:99:ALA:HB2     | 2.13                     | 0.49              |
| 2:B:297:THR:HB     | 2:B:300:GLU:H      | 1.78                     | 0.49              |
| 2:B:486:LEU:O      | 2:B:488:PRO:HD3    | 2.12                     | 0.49              |
| 22:B:1010:CLA:HED3 | 22:B:1011:CLA:CMA  | 2.43                     | 0.49              |
| 22:B:1020:CLA:H111 | 22:B:1020:CLA:H162 | 1.95                     | 0.49              |
| 25:B:1047:BCR:H392 | 25:B:1047:BCR:C22  | 2.35                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:70:PHE:CD1     | 10:K:26:PRO:HG3    | 2.48                     | 0.49              |
| 3:C:181:PHE:O      | 3:C:182:PHE:HD2    | 1.96                     | 0.49              |
| 3:C:314:ALA:HB1    | 3:C:351:PHE:HD1    | 1.78                     | 0.49              |
| 3:C:316:THR:HG21   | 16:V:74:THR:HG23   | 1.94                     | 0.49              |
| 3:C:437:PHE:O      | 3:C:440:GLY:N      | 2.46                     | 0.49              |
| 22:C:1030:CLA:HBD  | 22:C:1030:CLA:HAA1 | 1.95                     | 0.49              |
| 4:D:14:TRP:CD1     | 4:D:14:TRP:C       | 2.91                     | 0.49              |
| 4:D:16:ASP:O       | 4:D:20:ASP:N       | 2.45                     | 0.49              |
| 4:D:33:SER:OG      | 4:D:128:ARG:HG2    | 2.12                     | 0.49              |
| 4:D:88:SER:HB2     | 5:E:69:ARG:NH2     | 2.28                     | 0.49              |
| 4:D:194:ASN:C      | 4:D:194:ASN:OD1    | 2.55                     | 0.49              |
| 4:D:302:GLU:O      | 4:D:305:ALA:HB3    | 2.13                     | 0.49              |
| 22:D:1005:CLA:H202 | 22:D:1005:CLA:C15  | 2.42                     | 0.49              |
| 7:H:4:ARG:O        | 7:H:5:THR:CG2      | 2.60                     | 0.49              |
| 8:I:1:MET:C        | 8:I:3:THR:N        | 2.71                     | 0.49              |
| 8:I:10:ILE:HD13    | 8:I:10:ILE:N       | 2.28                     | 0.49              |
| 13:O:148:VAL:HA    | 13:O:172:PHE:CE2   | 2.47                     | 0.49              |
| 15:U:25:ILE:HD11   | 15:U:34:ALA:O      | 2.13                     | 0.49              |
| 16:V:70:GLY:O      | 16:V:157:GLY:O     | 2.30                     | 0.49              |
| 16:V:109:ASP:OD1   | 16:V:111:GLU:HG3   | 2.12                     | 0.49              |
| 20:Z:53:VAL:HG12   | 20:Z:57:LEU:HD12   | 1.95                     | 0.49              |
| 1:a:5101:SER:O     | 1:a:5102:LEU:C     | 2.56                     | 0.49              |
| 1:a:5129:ARG:O     | 4:d:5256:ILE:HD13  | 2.13                     | 0.49              |
| 1:a:5258:LEU:HD21  | 4:d:5129:GLN:HG2   | 1.95                     | 0.49              |
| 1:a:5323:ARG:NE    | 4:d:5332:GLN:HE22  | 2.11                     | 0.49              |
| 2:b:5103:LEU:O     | 2:b:5104:SER:C     | 2.56                     | 0.49              |
| 2:b:5195:PRO:O     | 2:b:5196:GLY:C     | 2.54                     | 0.49              |
| 2:b:5278:SER:CB    | 2:b:5281:GLN:HG2   | 2.27                     | 0.49              |
| 2:b:5355:PHE:HD2   | 2:b:5355:PHE:N     | 2.11                     | 0.49              |
| 22:b:6021:CLA:O1A  | 22:b:6021:CLA:O2D  | 2.30                     | 0.49              |
| 29:b:6058:DGD:HE5  | 29:b:6058:DGD:HD61 | 1.93                     | 0.49              |
| 3:c:5059:LEU:HD21  | 10:k:5032:PHE:CG   | 2.47                     | 0.49              |
| 3:c:5060:ILE:HG22  | 22:k:6034:CLA:CMD  | 2.42                     | 0.49              |
| 3:c:5088:LEU:CD1   | 22:c:6027:CLA:HBC2 | 2.42                     | 0.49              |
| 3:c:5117:VAL:HG11  | 22:c:6027:CLA:H11  | 1.95                     | 0.49              |
| 3:c:5270:ALA:O     | 3:c:5273:SER:HB3   | 2.12                     | 0.49              |
| 4:d:5191:TRP:HH2   | 4:d:5285:GLY:HA3   | 1.77                     | 0.49              |
| 4:d:5261:PHE:HB2   | 24:d:6042:PQ9:C10  | 2.43                     | 0.49              |
| 4:d:5262:SER:O     | 4:d:5263:ASN:CB    | 2.61                     | 0.49              |
| 7:h:5018:TYR:C     | 7:h:5018:TYR:CD2   | 2.90                     | 0.49              |
| 7:h:5038:PHE:CZ    | 7:h:5042:LEU:HD21  | 2.47                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:o:5239:GLY:O   | 13:o:5265:PHE:N    | 2.44                     | 0.49              |
| 17:x:5019:PHE:O   | 17:x:5020:PHE:C    | 2.52                     | 0.49              |
| 18:y:5043:ARG:N   | 18:y:5043:ARG:NE   | 2.61                     | 0.49              |
| 1:A:76:ASN:ND2    | 11:L:33:SER:CB     | 2.67                     | 0.48              |
| 1:A:78:ILE:N      | 1:A:78:ILE:CD1     | 2.76                     | 0.48              |
| 1:A:195:HIS:CE1   | 1:A:197:PHE:HB2    | 2.48                     | 0.48              |
| 1:A:303:ASN:OD1   | 1:A:322:ASN:ND2    | 2.46                     | 0.48              |
| 2:B:149:LEU:CD2   | 22:B:1011:CLA:HBC1 | 2.43                     | 0.48              |
| 2:B:174:LEU:CD2   | 2:B:312:TYR:CE1    | 2.95                     | 0.48              |
| 2:B:327:THR:HG23  | 11:L:37:ASN:ND2    | 2.28                     | 0.48              |
| 2:B:475:PHE:C     | 2:B:477:ASP:N      | 2.69                     | 0.48              |
| 22:B:1019:CLA:CBA | 22:B:1019:CLA:CBD  | 2.92                     | 0.48              |
| 3:C:284:PHE:HE1   | 3:C:431:PHE:CD2    | 2.31                     | 0.48              |
| 3:C:311:GLN:O     | 3:C:314:ALA:HB3    | 2.13                     | 0.48              |
| 22:C:1028:CLA:H18 | 29:C:1056:DGD:HA51 | 1.94                     | 0.48              |
| 22:C:1035:CLA:CMB | 25:C:1052:BCR:C27  | 2.90                     | 0.48              |
| 4:D:31:GLY:C      | 4:D:33:SER:N       | 2.66                     | 0.48              |
| 4:D:54:PHE:CB     | 5:E:47:PHE:CD1     | 2.96                     | 0.48              |
| 22:D:1005:CLA:CBA | 24:D:1042:PQ9:H412 | 2.38                     | 0.48              |
| 13:O:236:GLU:C    | 13:O:237:ILE:HG22  | 2.37                     | 0.48              |
| 20:Z:14:ILE:O     | 20:Z:18:VAL:HG23   | 2.13                     | 0.48              |
| 20:Z:15:LEU:HD11  | 20:Z:46:LEU:HG     | 1.95                     | 0.48              |
| 1:a:5111:PRO:HG2  | 1:a:5112:TYR:N     | 2.28                     | 0.48              |
| 1:a:5115:ILE:HG21 | 1:a:5174:LEU:HD13  | 1.93                     | 0.48              |
| 1:a:5187:GLN:NE2  | 1:a:5193:LEU:HB2   | 2.27                     | 0.48              |
| 1:a:5187:GLN:O    | 1:a:5191:ASN:N     | 2.37                     | 0.48              |
| 1:a:5311:GLY:O    | 1:a:5312:ASN:C     | 2.55                     | 0.48              |
| 1:a:5321:ILE:HD11 | 4:d:5176:ALA:CB    | 2.18                     | 0.48              |
| 2:b:5057:ARG:C    | 2:b:5059:GLY:H     | 2.21                     | 0.48              |
| 2:b:5090:PHE:CZ   | 2:b:5098:LEU:HD12  | 2.48                     | 0.48              |
| 2:b:5162:PHE:CD2  | 22:b:6014:CLA:HBC1 | 2.48                     | 0.48              |
| 2:b:5327:THR:HG23 | 11:l:5037:ASN:ND2  | 2.28                     | 0.48              |
| 3:c:5250:TRP:CD1  | 3:c:5250:TRP:C     | 2.90                     | 0.48              |
| 3:c:5284:PHE:HE1  | 3:c:5431:PHE:CD2   | 2.31                     | 0.48              |
| 3:c:5324:LEU:HD11 | 15:u:5042:TYR:OH   | 2.13                     | 0.48              |
| 3:c:5428:THR:O    | 3:c:5429:SER:C     | 2.56                     | 0.48              |
| 4:d:5031:GLY:C    | 4:d:5033:SER:N     | 2.66                     | 0.48              |
| 4:d:5048:TRP:CZ2  | 4:d:5052:THR:HG21  | 2.47                     | 0.48              |
| 4:d:5286:VAL:O    | 4:d:5287:VAL:C     | 2.56                     | 0.48              |
| 22:d:6008:CLA:HHC | 22:d:6008:CLA:CBB  | 2.19                     | 0.48              |
| 5:e:5023:HIS:HB3  | 5:e:5027:ILE:HD13  | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5172:PHE:CG   | 13:o:5221:GLY:HA3  | 2.48                     | 0.48              |
| 1:A:84:PRO:HA      | 1:A:112:TYR:CG     | 2.48                     | 0.48              |
| 1:A:284:TRP:O      | 1:A:285:PHE:C      | 2.56                     | 0.48              |
| 25:A:1044:BCR:HC7  | 8:I:15:PHE:HZ      | 1.78                     | 0.48              |
| 2:B:18:ARG:NH1     | 11:L:4:ASN:HB3     | 2.28                     | 0.48              |
| 2:B:355:PHE:CD2    | 2:B:355:PHE:N      | 2.81                     | 0.48              |
| 2:B:384:ARG:CD     | 15:U:102:LEU:HD21  | 2.42                     | 0.48              |
| 22:B:1010:CLA:O2D  | 22:B:1010:CLA:O1A  | 2.30                     | 0.48              |
| 3:C:50:LEU:CD2     | 3:C:51:GLY:HA2     | 2.43                     | 0.48              |
| 3:C:149:TYR:O      | 3:C:150:ASP:HB2    | 2.13                     | 0.48              |
| 3:C:457:LYS:HZ2    | 4:D:228:GLY:HA2    | 1.75                     | 0.48              |
| 3:C:459:ILE:N      | 4:D:224:GLN:H      | 2.08                     | 0.48              |
| 22:C:1035:CLA:H93  | 25:C:1052:BCR:C40  | 2.42                     | 0.48              |
| 4:D:53:THR:CG2     | 4:D:67:TYR:HD2     | 2.26                     | 0.48              |
| 4:D:319:LEU:O      | 4:D:323:GLU:HG3    | 2.13                     | 0.48              |
| 24:D:1042:PQ9:C24  | 28:L:1061:MGE:CGB  | 2.81                     | 0.48              |
| 7:H:38:PHE:O       | 7:H:41:PHE:HB3     | 2.14                     | 0.48              |
| 11:L:5:PRO:HG2     | 11:L:6:ASN:H       | 1.78                     | 0.48              |
| 13:O:172:PHE:CG    | 13:O:221:GLY:HA3   | 2.48                     | 0.48              |
| 16:V:148:GLU:N     | 16:V:149:PRO:HD2   | 2.29                     | 0.48              |
| 20:Z:37:LYS:HG3    | 20:Z:38:GLN:N      | 2.28                     | 0.48              |
| 1:a:5033:PHE:HB2   | 1:a:5129:ARG:HB2   | 1.94                     | 0.48              |
| 1:a:5202:VAL:HG22  | 1:a:5206:PHE:HD1   | 1.78                     | 0.48              |
| 1:a:5225:ARG:CB    | 2:b:5484:PRO:HD3   | 2.43                     | 0.48              |
| 2:b:5147:GLY:HA2   | 2:b:5150:CYS:HB3   | 1.95                     | 0.48              |
| 2:b:5308:LYS:HG2   | 2:b:5312:TYR:HE2   | 1.78                     | 0.48              |
| 22:b:6022:CLA:H11  | 22:b:6022:CLA:C20  | 2.43                     | 0.48              |
| 3:c:5149:TYR:O     | 3:c:5150:ASP:HB2   | 2.13                     | 0.48              |
| 3:c:5316:THR:HG21  | 16:v:5074:THR:HG23 | 1.94                     | 0.48              |
| 8:i:5016:VAL:O     | 8:i:5020:VAL:CG2   | 2.61                     | 0.48              |
| 10:k:5033:PHE:HA   | 22:k:6034:CLA:HMA1 | 1.95                     | 0.48              |
| 28:l:6061:MGE:H3B1 | 28:l:6061:MGE:H6B2 | 1.58                     | 0.48              |
| 12:m:5018:PRO:HG2  | 12:m:5019:SER:H    | 1.77                     | 0.48              |
| 12:m:5032:GLN:HA   | 12:m:5032:GLN:NE2  | 2.27                     | 0.48              |
| 13:o:5151:LEU:HD12 | 13:o:5171:GLU:O    | 2.13                     | 0.48              |
| 15:u:5051:LYS:HG3  | 15:u:5052:ASN:N    | 2.23                     | 0.48              |
| 16:v:5096:GLU:O    | 16:v:5097:GLY:C    | 2.55                     | 0.48              |
| 1:A:258:LEU:O      | 1:A:259:ILE:HG13   | 2.12                     | 0.48              |
| 1:A:308:ASP:OD1    | 1:A:312:ASN:O      | 2.31                     | 0.48              |
| 1:A:323:ARG:NE     | 4:D:332:GLN:HE22   | 2.11                     | 0.48              |
| 23:A:1038:PHO:C4C  | 4:D:209:LEU:HG     | 2.43                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:66:MET:HE3     | 2:B:96:VAL:HB      | 1.94                     | 0.48              |
| 2:B:137:LYS:HG3    | 2:B:217:ILE:HA     | 1.95                     | 0.48              |
| 2:B:257:TRP:CD2    | 4:D:291:LEU:HD22   | 2.48                     | 0.48              |
| 2:B:271:THR:HG23   | 2:B:274:GLN:CB     | 2.42                     | 0.48              |
| 2:B:324:LEU:HA     | 4:D:293:LEU:CD2    | 2.31                     | 0.48              |
| 2:B:451:PHE:C      | 2:B:451:PHE:CD2    | 2.90                     | 0.48              |
| 22:B:1015:CLA:OBD  | 22:B:1015:CLA:CED  | 2.38                     | 0.48              |
| 3:C:155:ASN:C      | 3:C:158:THR:HG22   | 2.38                     | 0.48              |
| 3:C:315:MET:HE2    | 3:C:319:ILE:HG13   | 1.95                     | 0.48              |
| 3:C:406:SER:CB     | 29:C:1056:DGD:HE1  | 2.39                     | 0.48              |
| 4:D:24:ARG:HA      | 4:D:24:ARG:HE      | 1.77                     | 0.48              |
| 4:D:302:GLU:HA     | 4:D:305:ALA:HB2    | 1.96                     | 0.48              |
| 4:D:308:ASP:C      | 4:D:310:GLU:N      | 2.72                     | 0.48              |
| 4:D:342:PRO:HD2    | 4:D:345:VAL:HG21   | 1.94                     | 0.48              |
| 22:D:1008:CLA:H61  | 22:D:1008:CLA:H101 | 1.69                     | 0.48              |
| 5:E:13:ILE:CG1     | 5:E:19:TYR:HB2     | 2.43                     | 0.48              |
| 6:F:19:ARG:NH2     | 6:F:20:TRP:CD1     | 2.81                     | 0.48              |
| 13:O:69:LEU:HD11   | 13:O:71:LEU:CD2    | 2.43                     | 0.48              |
| 16:V:35:THR:CA     | 16:V:46:THR:HA     | 2.43                     | 0.48              |
| 16:V:39:ASN:HD22   | 16:V:40:SER:H      | 1.59                     | 0.48              |
| 16:V:160:LYS:O     | 16:V:163:TYR:HB2   | 2.13                     | 0.48              |
| 1:a:5055:ALA:H     | 1:a:5070:SER:HB2   | 1.77                     | 0.48              |
| 1:a:5265:PHE:HD1   | 1:a:5271:LEU:HA    | 1.79                     | 0.48              |
| 1:a:5322:ASN:OD1   | 3:c:5412:THR:HB    | 2.12                     | 0.48              |
| 25:a:6044:BCR:HC7  | 8:i:5015:PHE:HZ    | 1.78                     | 0.48              |
| 2:b:5120:LEU:HD23  | 2:b:5120:LEU:N     | 2.28                     | 0.48              |
| 2:b:5122:LEU:HD21  | 7:h:5011:LEU:HB2   | 1.95                     | 0.48              |
| 22:b:6009:CLA:OBD  | 22:b:6010:CLA:CBB  | 2.55                     | 0.48              |
| 22:b:6018:CLA:OBD  | 22:b:6018:CLA:H13  | 2.14                     | 0.48              |
| 22:b:6021:CLA:O1A  | 22:b:6021:CLA:C2   | 2.60                     | 0.48              |
| 3:c:5075:PHE:HD1   | 3:c:5086:LEU:HD11  | 1.78                     | 0.48              |
| 3:c:5181:PHE:O     | 3:c:5182:PHE:HD2   | 1.96                     | 0.48              |
| 3:c:5212:TYR:HB3   | 3:c:5223:TRP:O     | 2.13                     | 0.48              |
| 3:c:5351:PHE:CZ    | 3:c:5366:LEU:HD11  | 2.48                     | 0.48              |
| 4:d:5147:SER:O     | 4:d:5148:ALA:C     | 2.55                     | 0.48              |
| 4:d:5317:LYS:HG2   | 27:d:6064:IOD:I    | 2.82                     | 0.48              |
| 4:d:5319:LEU:O     | 4:d:5323:GLU:HG3   | 2.13                     | 0.48              |
| 28:d:6062:MGE:H231 | 11:l:5026:VAL:CG2  | 2.44                     | 0.48              |
| 7:h:5034:PHE:CE2   | 22:h:6017:CLA:HAC1 | 2.48                     | 0.48              |
| 12:m:5008:PHE:O    | 12:m:5012:ALA:HB3  | 2.13                     | 0.48              |
| 13:o:5128:ASP:OD1  | 13:o:5149:LYS:HG2  | 2.13                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5147:THR:OG1  | 13:o:5149:LYS:HG3  | 2.13                     | 0.48              |
| 13:o:5214:LYS:HE3  | 13:o:5251:MET:CG   | 2.34                     | 0.48              |
| 14:t:5019:PHE:N    | 14:t:5019:PHE:HD2  | 2.10                     | 0.48              |
| 15:u:5035:PHE:HD1  | 15:u:5046:ALA:HB2  | 1.78                     | 0.48              |
| 16:v:5070:GLY:O    | 16:v:5157:GLY:O    | 2.30                     | 0.48              |
| 16:v:5114:ILE:CD1  | 31:v:6041:HEM:HBD2 | 2.43                     | 0.48              |
| 20:z:5014:ILE:O    | 20:z:5018:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:119:PHE:C      | 1:A:121:LEU:N      | 2.71                     | 0.48              |
| 1:A:129:ARG:O      | 4:D:256:ILE:HD13   | 2.13                     | 0.48              |
| 1:A:200:LEU:CD2    | 29:C:1057:DGD:HBW2 | 2.43                     | 0.48              |
| 1:A:255:PHE:O      | 1:A:256:GLY:C      | 2.57                     | 0.48              |
| 2:B:5:TRP:CD1      | 2:B:5:TRP:N        | 2.76                     | 0.48              |
| 2:B:373:LYS:H      | 2:B:373:LYS:HG2    | 1.32                     | 0.48              |
| 22:B:1022:CLA:H62  | 22:B:1022:CLA:H141 | 1.75                     | 0.48              |
| 3:C:46:SER:OG      | 3:C:141:GLU:CB     | 2.60                     | 0.48              |
| 3:C:87:ILE:O       | 3:C:90:PRO:CG      | 2.61                     | 0.48              |
| 3:C:155:ASN:O      | 3:C:158:THR:CG2    | 2.61                     | 0.48              |
| 3:C:414:ILE:CG2    | 3:C:415:ASN:N      | 2.76                     | 0.48              |
| 3:C:449:ARG:HB2    | 22:C:1029:CLA:CED  | 2.43                     | 0.48              |
| 4:D:250:ASN:C      | 4:D:252:PHE:N      | 2.72                     | 0.48              |
| 25:D:1050:BCR:C20  | 28:D:1059:MGE:C5A  | 2.88                     | 0.48              |
| 25:K:1051:BCR:C8   | 25:K:1051:BCR:H311 | 2.44                     | 0.48              |
| 11:L:36:PHE:CZ     | 14:T:2:GLU:HB3     | 2.48                     | 0.48              |
| 12:M:32:GLN:HE22   | 12:m:5034:LYS:HA   | 1.79                     | 0.48              |
| 13:O:162:ILE:CD1   | 13:O:269:ILE:HD12  | 2.43                     | 0.48              |
| 16:V:160:LYS:N     | 16:V:163:TYR:CE1   | 2.78                     | 0.48              |
| 18:Y:19:ILE:HG22   | 18:Y:20:ALA:N      | 2.28                     | 0.48              |
| 1:a:5065:GLU:OE1   | 4:d:5312:GLU:OE2   | 2.31                     | 0.48              |
| 1:a:5308:ASP:OD1   | 1:a:5312:ASN:O     | 2.31                     | 0.48              |
| 2:b:5025:MET:O     | 2:b:5028:ALA:N     | 2.47                     | 0.48              |
| 2:b:5109:LEU:C     | 2:b:5111:ALA:N     | 2.66                     | 0.48              |
| 2:b:5456:ALA:HB1   | 29:b:6058:DGD:CHB  | 2.28                     | 0.48              |
| 29:b:6058:DGD:HBF2 | 29:b:6058:DGD:HBG3 | 1.83                     | 0.48              |
| 3:c:5049:LEU:CD1   | 22:c:6035:CLA:HMA3 | 2.43                     | 0.48              |
| 3:c:5070:PHE:CD1   | 10:k:5026:PRO:HG3  | 2.48                     | 0.48              |
| 3:c:5087:ILE:O     | 3:c:5091:HIS:CE1   | 2.66                     | 0.48              |
| 3:c:5119:LEU:C     | 3:c:5119:LEU:HD12  | 2.37                     | 0.48              |
| 3:c:5155:ASN:C     | 3:c:5158:THR:HG22  | 2.38                     | 0.48              |
| 22:c:6035:CLA:H93  | 25:k:6052:BCR:C40  | 2.42                     | 0.48              |
| 4:d:5054:PHE:CB    | 5:e:5047:PHE:CD1   | 2.96                     | 0.48              |
| 4:d:5058:TRP:NE1   | 5:e:5064:PRO:HD2   | 2.21                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5223:PHE:CZ    | 4:d:5245:SER:HB2   | 2.49                     | 0.48              |
| 25:d:6050:BCR:H363 | 6:f:5030:THR:HG23  | 1.94                     | 0.48              |
| 28:d:6062:MGE:O1A  | 28:d:6062:MGE:C3B  | 2.60                     | 0.48              |
| 9:j:5008:ILE:HD12  | 9:j:5008:ILE:N     | 2.29                     | 0.48              |
| 11:l:5036:PHE:CZ   | 14:t:5002:GLU:HB3  | 2.48                     | 0.48              |
| 15:u:5061:VAL:HG12 | 15:u:5075:LEU:CD2  | 2.37                     | 0.48              |
| 20:z:5037:LYS:HG3  | 20:z:5038:GLN:N    | 2.28                     | 0.48              |
| 1:A:118:HIS:O      | 1:A:121:LEU:HB3    | 2.13                     | 0.48              |
| 1:A:184:ILE:CD1    | 4:D:186:GLN:HE22   | 2.26                     | 0.48              |
| 2:B:62:VAL:HG13    | 22:B:1013:CLA:HED2 | 1.95                     | 0.48              |
| 2:B:109:LEU:C      | 2:B:111:ALA:N      | 2.66                     | 0.48              |
| 2:B:113:TRP:C      | 2:B:115:TRP:N      | 2.69                     | 0.48              |
| 2:B:326:ARG:HH11   | 4:D:297:ASP:CA     | 2.11                     | 0.48              |
| 22:B:1019:CLA:HMD1 | 28:B:1060:MGE:H2G  | 1.96                     | 0.48              |
| 25:B:1047:BCR:C23  | 25:t:1046:BCR:H353 | 2.41                     | 0.48              |
| 3:C:46:SER:CB      | 3:C:141:GLU:N      | 2.77                     | 0.48              |
| 3:C:54:VAL:O       | 3:C:55:ALA:C       | 2.55                     | 0.48              |
| 3:C:212:TYR:HB3    | 3:C:223:TRP:O      | 2.13                     | 0.48              |
| 3:C:362:ARG:HH22   | 13:O:34:ASP:CG     | 2.20                     | 0.48              |
| 22:C:1026:CLA:H122 | 22:C:1026:CLA:C6   | 2.44                     | 0.48              |
| 4:D:106:GLN:C      | 4:D:108:GLY:N      | 2.72                     | 0.48              |
| 5:E:7:GLU:OE2      | 6:F:19:ARG:HB2     | 2.13                     | 0.48              |
| 8:I:16:VAL:O       | 8:I:20:VAL:CG2     | 2.61                     | 0.48              |
| 16:V:61:TYR:C      | 16:V:63:CYS:N      | 2.68                     | 0.48              |
| 1:a:5126:TYR:O     | 1:a:5126:TYR:CD2   | 2.58                     | 0.48              |
| 1:a:5224:ILE:HB    | 1:a:5245:THR:O     | 2.12                     | 0.48              |
| 2:b:5030:VAL:HG13  | 22:b:6013:CLA:CMD  | 2.43                     | 0.48              |
| 2:b:5040:TYR:O     | 2:b:5043:ALA:N     | 2.46                     | 0.48              |
| 2:b:5041:GLU:OE1   | 2:b:5061:PHE:N     | 2.35                     | 0.48              |
| 2:b:5054:PRO:O     | 2:b:5055:MET:C     | 2.57                     | 0.48              |
| 22:b:6013:CLA:HMB3 | 22:b:6014:CLA:H11  | 1.94                     | 0.48              |
| 22:b:6019:CLA:CBA  | 22:b:6019:CLA:CBF  | 2.92                     | 0.48              |
| 3:c:5050:LEU:CD2   | 3:c:5051:GLY:HA2   | 2.43                     | 0.48              |
| 3:c:5072:LEU:CD1   | 3:c:5112:PHE:HB2   | 2.43                     | 0.48              |
| 3:c:5311:GLN:O     | 3:c:5314:ALA:HB3   | 2.13                     | 0.48              |
| 3:c:5342:MET:HG2   | 3:c:5343:ARG:H     | 1.77                     | 0.48              |
| 25:c:6054:BCR:H24C | 25:c:6054:BCR:H371 | 1.64                     | 0.48              |
| 4:d:5015:PHE:CE1   | 4:d:5032:TRP:CZ2   | 2.98                     | 0.48              |
| 7:h:5040:VAL:O     | 7:h:5044:ILE:HG12  | 2.13                     | 0.48              |
| 13:o:5200:LEU:HB3  | 13:o:5203:ALA:HB2  | 1.94                     | 0.48              |
| 15:u:5100:ASN:O    | 15:u:5100:ASN:OD1  | 2.32                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:v:5064:ALA:O    | 16:v:5068:VAL:N    | 2.46                     | 0.48              |
| 1:A:96:ILE:HD12    | 22:A:1007:CLA:CMD  | 2.43                     | 0.48              |
| 1:A:142:TRP:CH2    | 26:A:1063:LHG:HC5  | 2.47                     | 0.48              |
| 1:A:279:ARG:CG     | 4:D:212:ALA:HB2    | 2.43                     | 0.48              |
| 2:B:18:ARG:HH11    | 11:L:4:ASN:HD22    | 1.60                     | 0.48              |
| 2:B:25:MET:O       | 2:B:28:ALA:N       | 2.47                     | 0.48              |
| 2:B:49:ASP:HB2     | 13:o:5083:LYS:HE3  | 1.94                     | 0.48              |
| 2:B:54:PRO:O       | 2:B:55:MET:C       | 2.57                     | 0.48              |
| 2:B:83:GLU:HG2     | 2:B:86:ILE:CD1     | 2.32                     | 0.48              |
| 2:B:103:LEU:O      | 2:B:104:SER:C      | 2.56                     | 0.48              |
| 2:B:135:LEU:HA     | 2:B:138:MET:HB3    | 1.95                     | 0.48              |
| 3:C:60:ILE:HA      | 22:K:1034:CLA:HMD3 | 1.96                     | 0.48              |
| 3:C:176:VAL:HA     | 3:C:234:VAL:HG23   | 1.95                     | 0.48              |
| 3:C:272:LEU:HD12   | 3:C:272:LEU:O      | 2.13                     | 0.48              |
| 3:C:370:ARG:HG3    | 3:C:371:GLY:N      | 2.28                     | 0.48              |
| 3:C:465:PRO:O      | 3:C:469:MET:HG3    | 2.13                     | 0.48              |
| 22:C:1032:CLA:H3A  | 22:C:1032:CLA:HBA2 | 1.40                     | 0.48              |
| 4:D:250:ASN:CG     | 4:D:251:ARG:N      | 2.70                     | 0.48              |
| 25:D:1050:BCR:H363 | 6:F:30:THR:HG23    | 1.94                     | 0.48              |
| 5:E:47:PHE:O       | 5:E:49:THR:N       | 2.41                     | 0.48              |
| 7:H:7:LEU:HA       | 7:H:10:ILE:HD12    | 1.94                     | 0.48              |
| 8:I:1:MET:O        | 8:I:3:THR:N        | 2.47                     | 0.48              |
| 11:L:8:GLN:HE21    | 11:L:8:GLN:N       | 2.07                     | 0.48              |
| 13:O:129:PHE:CD2   | 13:O:129:PHE:C     | 2.92                     | 0.48              |
| 13:O:147:THR:OG1   | 13:O:149:LYS:HG3   | 2.13                     | 0.48              |
| 15:U:85:THR:O      | 15:U:86:GLU:C      | 2.56                     | 0.48              |
| 15:U:100:ASN:OD1   | 15:U:100:ASN:O     | 2.32                     | 0.48              |
| 1:a:5197:PHE:HE1   | 1:a:5285:PHE:CD2   | 2.23                     | 0.48              |
| 1:a:5257:ARG:O     | 1:a:5259:ILE:N     | 2.46                     | 0.48              |
| 2:b:5137:LYS:HG3   | 2:b:5217:ILE:HA    | 1.95                     | 0.48              |
| 2:b:5215:PHE:C     | 2:b:5215:PHE:HD2   | 2.20                     | 0.48              |
| 3:c:5465:PRO:O     | 3:c:5469:MET:HG3   | 2.13                     | 0.48              |
| 22:c:6028:CLA:H111 | 22:c:6028:CLA:H152 | 1.71                     | 0.48              |
| 22:c:6030:CLA:CMB  | 22:c:6031:CLA:C4B  | 2.85                     | 0.48              |
| 22:c:6032:CLA:H12  | 22:c:6035:CLA:C3C  | 2.44                     | 0.48              |
| 4:d:5101:PHE:O     | 4:d:5101:PHE:CG    | 2.65                     | 0.48              |
| 4:d:5250:ASN:C     | 4:d:5252:PHE:N     | 2.72                     | 0.48              |
| 24:d:6042:PQ9:H312 | 24:d:6042:PQ9:H27  | 1.57                     | 0.48              |
| 9:j:5010:LEU:H     | 9:j:5010:LEU:CD1   | 2.10                     | 0.48              |
| 10:k:5028:ILE:HA   | 10:k:5031:LEU:CD1  | 2.43                     | 0.48              |
| 13:o:5069:LEU:HD12 | 13:o:5070:CYS:N    | 2.28                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5129:PHE:CD2  | 13:o:5129:PHE:C    | 2.92                     | 0.48              |
| 13:o:5163:THR:HG23 | 13:o:5165:SER:H    | 1.78                     | 0.48              |
| 14:t:5001:MET:HG2  | 14:t:5002:GLU:N    | 2.27                     | 0.48              |
| 18:y:5019:ILE:HG22 | 18:y:5020:ALA:N    | 2.28                     | 0.48              |
| 1:A:161:TYR:CZ     | 1:A:186:PHE:HE2    | 2.31                     | 0.48              |
| 1:A:272:HIS:NE2    | 4:D:214:HIS:NE2    | 2.61                     | 0.48              |
| 1:A:302:PHE:N      | 1:A:302:PHE:CD1    | 2.82                     | 0.48              |
| 1:A:340:PRO:HG3    | 3:C:317:PHE:CZ     | 2.48                     | 0.48              |
| 22:A:1006:CLA:HED3 | 4:D:175:VAL:HG13   | 1.96                     | 0.48              |
| 2:B:8:VAL:HG21     | 22:B:1022:CLA:C3D  | 2.44                     | 0.48              |
| 2:B:27:THR:HG22    | 2:B:107:LEU:HD13   | 1.96                     | 0.48              |
| 2:B:162:PHE:CD2    | 22:B:1014:CLA:HBC1 | 2.48                     | 0.48              |
| 3:C:263:ALA:HB1    | 3:C:264:PHE:CD2    | 2.45                     | 0.48              |
| 3:C:305:THR:O      | 3:C:306:GLY:C      | 2.56                     | 0.48              |
| 22:C:1037:CLA:H8   | 22:C:1037:CLA:H142 | 1.96                     | 0.48              |
| 4:D:127:LEU:O      | 4:D:130:PHE:N      | 2.45                     | 0.48              |
| 4:D:155:SER:HA     | 4:D:159:ILE:CB     | 2.44                     | 0.48              |
| 4:D:183:LEU:HD23   | 4:D:183:LEU:N      | 2.14                     | 0.48              |
| 9:J:25:VAL:HA      | 9:J:28:PHE:CD2     | 2.43                     | 0.48              |
| 12:M:34:LYS:HG3    | 11:I:5009:PRO:CB   | 2.43                     | 0.48              |
| 13:O:128:ASP:OD1   | 13:O:149:LYS:HG2   | 2.13                     | 0.48              |
| 13:O:163:THR:O     | 13:O:165:SER:N     | 2.46                     | 0.48              |
| 14:T:1:MET:HG2     | 14:T:2:GLU:N       | 2.27                     | 0.48              |
| 15:U:78:ASN:O      | 15:U:80:GLU:N      | 2.46                     | 0.48              |
| 16:V:36:VAL:HG21   | 16:V:146:LEU:HD12  | 1.95                     | 0.48              |
| 16:V:154:ASP:O     | 16:V:156:TRP:N     | 2.47                     | 0.48              |
| 18:Y:39:LEU:CD2    | 20:Z:28:ALA:HB1    | 2.42                     | 0.48              |
| 19:N:1:UNK:O       | 19:N:2:UNK:CB      | 2.62                     | 0.48              |
| 1:a:5086:SER:C     | 1:a:5088:ALA:N     | 2.68                     | 0.48              |
| 1:a:5124:SER:OG    | 1:a:5155:PHE:HE2   | 1.97                     | 0.48              |
| 1:a:5184:ILE:CD1   | 4:d:5186:GLN:HE22  | 2.26                     | 0.48              |
| 1:a:5200:LEU:CD2   | 29:c:6057:DGD:HBW2 | 2.43                     | 0.48              |
| 1:a:5269:ARG:HG3   | 4:d:5235:PHE:HB2   | 1.93                     | 0.48              |
| 1:a:5290:ILE:HG22  | 1:a:5291:SER:H     | 1.78                     | 0.48              |
| 2:b:5095:GLY:O     | 2:b:5099:ALA:HB2   | 2.13                     | 0.48              |
| 22:b:6021:CLA:C11  | 28:b:6060:MGE:H132 | 2.42                     | 0.48              |
| 3:c:5046:SER:CB    | 3:c:5141:GLU:N     | 2.77                     | 0.48              |
| 3:c:5060:ILE:HA    | 22:k:6034:CLA:HMD3 | 1.96                     | 0.48              |
| 3:c:5272:LEU:O     | 3:c:5272:LEU:HD12  | 2.13                     | 0.48              |
| 22:c:6027:CLA:H141 | 25:z:6053:BCR:H333 | 1.94                     | 0.48              |
| 4:d:5127:LEU:O     | 4:d:5130:PHE:N     | 2.45                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:e:5079:PHE:C     | 5:e:5083:LEU:HD13  | 2.38                     | 0.48              |
| 7:h:5038:PHE:O     | 7:h:5041:PHE:HB3   | 2.14                     | 0.48              |
| 8:i:5001:MET:C     | 8:i:5003:THR:N     | 2.71                     | 0.48              |
| 10:k:5032:PHE:CD1  | 25:k:6052:BCR:C38  | 2.86                     | 0.48              |
| 13:o:5069:LEU:HD11 | 13:o:5071:LEU:CD2  | 2.43                     | 0.48              |
| 13:o:5215:ARG:H    | 13:o:5215:ARG:HD3  | 1.78                     | 0.48              |
| 16:v:5036:VAL:HG21 | 16:v:5146:LEU:HD12 | 1.95                     | 0.48              |
| 19:n:5001:UNK:O    | 19:n:5002:UNK:CB   | 2.62                     | 0.48              |
| 1:A:24:THR:HG23    | 3:C:469:MET:HE3    | 1.95                     | 0.48              |
| 1:A:124:SER:OG     | 1:A:155:PHE:HE2    | 1.97                     | 0.48              |
| 1:A:202:VAL:HG22   | 1:A:206:PHE:HD1    | 1.78                     | 0.48              |
| 1:A:202:VAL:HG23   | 22:A:1003:CLA:HMB2 | 1.95                     | 0.48              |
| 1:A:214:MET:HE3    | 1:A:255:PHE:CZ     | 2.49                     | 0.48              |
| 1:A:311:GLY:O      | 1:A:312:ASN:C      | 2.55                     | 0.48              |
| 2:B:108:PHE:C      | 2:B:111:ALA:HB3    | 2.38                     | 0.48              |
| 2:B:460:LEU:HD23   | 4:D:280:TRP:CZ3    | 2.49                     | 0.48              |
| 22:B:1021:CLA:HMD2 | 22:B:1022:CLA:CBB  | 2.34                     | 0.48              |
| 22:B:1022:CLA:C3D  | 22:B:1022:CLA:H201 | 2.44                     | 0.48              |
| 22:B:1022:CLA:H203 | 22:B:1022:CLA:C2   | 2.44                     | 0.48              |
| 25:B:1048:BCR:C8   | 25:B:1048:BCR:C33  | 2.81                     | 0.48              |
| 3:C:87:ILE:O       | 3:C:91:HIS:CE1     | 2.66                     | 0.48              |
| 3:C:168:LEU:C      | 3:C:170:ILE:N      | 2.71                     | 0.48              |
| 3:C:305:THR:HG23   | 3:C:308:GLU:H      | 1.79                     | 0.48              |
| 29:C:1056:DGD:HBF1 | 29:C:1056:DGD:HB81 | 1.95                     | 0.48              |
| 4:D:49:LEU:HD13    | 25:D:1050:BCR:C15  | 2.44                     | 0.48              |
| 4:D:302:GLU:OE1    | 13:O:186:LYS:HD3   | 2.14                     | 0.48              |
| 6:F:20:TRP:HE1     | 31:F:1040:HEM:CHD  | 2.27                     | 0.48              |
| 13:O:69:LEU:HD12   | 13:O:70:CYS:N      | 2.28                     | 0.48              |
| 14:T:18:PHE:CD1    | 25:T:6046:BCR:H332 | 2.48                     | 0.48              |
| 25:T:6046:BCR:H282 | 22:b:6015:CLA:HAC2 | 1.88                     | 0.48              |
| 15:U:17:LEU:O      | 15:U:17:LEU:HD23   | 2.13                     | 0.48              |
| 1:a:5024:THR:HG23  | 3:c:5469:MET:HE3   | 1.95                     | 0.48              |
| 1:a:5214:MET:HE3   | 1:a:5255:PHE:CZ    | 2.49                     | 0.48              |
| 1:a:5329:GLU:O     | 1:a:5332:HIS:ND1   | 2.47                     | 0.48              |
| 2:b:5002:GLY:HA2   | 11:l:5011:GLU:HB2  | 1.96                     | 0.48              |
| 2:b:5070:GLY:HA2   | 2:b:5178:VAL:HG21  | 1.96                     | 0.48              |
| 2:b:5135:LEU:HA    | 2:b:5138:MET:HB3   | 1.95                     | 0.48              |
| 3:c:5049:LEU:CD1   | 22:c:6035:CLA:CMA  | 2.88                     | 0.48              |
| 3:c:5314:ALA:HB1   | 3:c:5351:PHE:HD1   | 1.78                     | 0.48              |
| 22:c:6033:CLA:C14  | 22:c:6033:CLA:C17  | 2.68                     | 0.48              |
| 29:c:6055:DGD:C6A  | 29:c:6055:DGD:CAA  | 2.85                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:e:5027:ILE:HG13  | 31:f:6040:HEM:HMB1 | 1.95                     | 0.48              |
| 8:i:5001:MET:C     | 8:i:5003:THR:H     | 2.22                     | 0.48              |
| 8:i:5001:MET:O     | 8:i:5003:THR:N     | 2.47                     | 0.48              |
| 13:o:5052:ALA:O    | 13:o:5053:ARG:CB   | 2.62                     | 0.48              |
| 15:u:5078:ASN:O    | 15:u:5080:GLU:N    | 2.46                     | 0.48              |
| 16:v:5046:THR:O    | 16:v:5047:LEU:CB   | 2.58                     | 0.48              |
| 1:A:111:PRO:HG2    | 1:A:112:TYR:N      | 2.28                     | 0.48              |
| 22:A:1003:CLA:CED  | 22:A:1003:CLA:CGA  | 2.92                     | 0.48              |
| 24:A:1043:PQ9:H453 | 24:A:1043:PQ9:H401 | 1.96                     | 0.48              |
| 2:B:40:TYR:O       | 2:B:43:ALA:N       | 2.46                     | 0.48              |
| 2:B:334:ASP:OD2    | 2:B:334:ASP:N      | 2.32                     | 0.48              |
| 22:B:1023:CLA:H93  | 22:B:1024:CLA:H152 | 1.95                     | 0.48              |
| 3:C:117:VAL:HG11   | 22:C:1027:CLA:H12  | 1.94                     | 0.48              |
| 3:C:157:MET:HB3    | 22:C:1031:CLA:HBC1 | 1.95                     | 0.48              |
| 3:C:324:LEU:HD11   | 15:U:42:TYR:OH     | 2.13                     | 0.48              |
| 3:C:351:PHE:CZ     | 3:C:366:LEU:HD11   | 2.48                     | 0.48              |
| 3:C:440:GLY:O      | 3:C:441:HIS:C      | 2.56                     | 0.48              |
| 22:C:1037:CLA:HBA2 | 22:C:1037:CLA:H3A  | 1.44                     | 0.48              |
| 5:E:13:ILE:HD12    | 5:E:16:SER:CB      | 2.44                     | 0.48              |
| 10:K:21:LEU:O      | 10:K:22:VAL:C      | 2.57                     | 0.48              |
| 25:K:1051:BCR:H23C | 25:K:1051:BCR:H392 | 1.96                     | 0.48              |
| 12:M:20:VAL:HG22   | 12:m:5020:VAL:HG11 | 1.95                     | 0.48              |
| 1:a:5041:LEU:CD1   | 1:a:5119:PHE:HA    | 2.44                     | 0.48              |
| 1:a:5061:ASP:HB2   | 1:a:5063:ILE:CD1   | 2.44                     | 0.48              |
| 1:a:5078:ILE:N     | 1:a:5078:ILE:CD1   | 2.76                     | 0.48              |
| 1:a:5093:PHE:HB2   | 3:c:5218:PHE:CD2   | 2.47                     | 0.48              |
| 22:a:6006:CLA:HED3 | 4:d:5175:VAL:HG13  | 1.96                     | 0.48              |
| 22:a:6007:CLA:C6   | 22:a:6007:CLA:C11  | 2.92                     | 0.48              |
| 2:b:5025:MET:O     | 2:b:5026:HIS:C     | 2.56                     | 0.48              |
| 2:b:5122:LEU:HD21  | 7:h:5012:ARG:N     | 2.29                     | 0.48              |
| 2:b:5162:PHE:CD1   | 2:b:5162:PHE:C     | 2.92                     | 0.48              |
| 2:b:5309:LEU:O     | 2:b:5310:ALA:C     | 2.57                     | 0.48              |
| 2:b:5400:SER:HA    | 2:b:5410:THR:HG22  | 1.96                     | 0.48              |
| 2:b:5452:THR:HG22  | 4:d:5291:LEU:HD11  | 1.95                     | 0.48              |
| 2:b:5477:ASP:OD2   | 4:d:5134:ARG:NH1   | 2.43                     | 0.48              |
| 22:b:6010:CLA:HED3 | 22:b:6011:CLA:CMA  | 2.43                     | 0.48              |
| 3:c:5169:GLY:HA2   | 3:c:5241:GLY:HA2   | 1.96                     | 0.48              |
| 3:c:5212:TYR:O     | 3:c:5215:LYS:HB2   | 2.13                     | 0.48              |
| 3:c:5274:TYR:HB2   | 3:c:5275:SER:H     | 1.40                     | 0.48              |
| 4:d:5301:GLN:HE22  | 4:d:5313:THR:HG21  | 1.79                     | 0.48              |
| 22:d:6008:CLA:OBD  | 22:d:6008:CLA:HED3 | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k:5035:LEU:O    | 10:k:5037:PHE:N    | 2.46                     | 0.48              |
| 13:o:5059:ASP:HB2  | 13:o:5062:GLN:HB2  | 1.94                     | 0.48              |
| 16:v:5038:LEU:HA   | 16:v:5045:ILE:HD11 | 1.95                     | 0.48              |
| 16:v:5148:GLU:N    | 16:v:5149:PRO:HD2  | 2.29                     | 0.48              |
| 16:v:5154:ASP:C    | 16:v:5156:TRP:N    | 2.70                     | 0.48              |
| 1:A:128:GLY:C      | 1:A:130:GLN:N      | 2.72                     | 0.48              |
| 1:A:228:THR:CG2    | 1:A:229:GLU:H      | 2.10                     | 0.48              |
| 1:A:288:LEU:HD21   | 3:C:435:PHE:CD2    | 2.49                     | 0.48              |
| 22:A:1006:CLA:HBC1 | 4:D:182:LEU:CD2    | 2.41                     | 0.48              |
| 2:B:277:SER:C      | 2:B:279:TYR:N      | 2.71                     | 0.48              |
| 2:B:374:ASN:N      | 2:B:374:ASN:ND2    | 2.58                     | 0.48              |
| 22:B:1010:CLA:H151 | 29:B:1058:DGD:C8A  | 2.38                     | 0.48              |
| 22:B:1022:CLA:O1D  | 22:B:1022:CLA:C1   | 2.62                     | 0.48              |
| 22:B:1022:CLA:H11  | 22:B:1022:CLA:C20  | 2.43                     | 0.48              |
| 3:C:212:TYR:O      | 3:C:215:LYS:HB2    | 2.13                     | 0.48              |
| 3:C:342:MET:HB2    | 3:C:352:GLY:HA3    | 1.96                     | 0.48              |
| 4:D:251:ARG:HH22   | 4:D:255:GLN:NE2    | 2.10                     | 0.48              |
| 5:E:23:HIS:HB3     | 5:E:27:ILE:HD13    | 1.95                     | 0.48              |
| 1:a:5340:PRO:HG3   | 3:c:5317:PHE:CZ    | 2.48                     | 0.48              |
| 22:a:6006:CLA:HAA2 | 29:c:6057:DGD:HBN1 | 1.96                     | 0.48              |
| 2:b:5460:LEU:HD23  | 4:d:5280:TRP:CZ3   | 2.49                     | 0.48              |
| 22:b:6018:CLA:HBB2 | 22:h:6017:CLA:H2   | 1.96                     | 0.48              |
| 3:c:5054:VAL:O     | 3:c:5055:ALA:C     | 2.55                     | 0.48              |
| 3:c:5292:PHE:CE1   | 29:c:6055:DGD:HD1  | 2.49                     | 0.48              |
| 3:c:5305:THR:O     | 3:c:5306:GLY:C     | 2.56                     | 0.48              |
| 3:c:5370:ARG:HG3   | 3:c:5371:GLY:N     | 2.28                     | 0.48              |
| 4:d:5299:ILE:C     | 4:d:5301:GLN:N     | 2.72                     | 0.48              |
| 4:d:5302:GLU:OE1   | 13:o:5186:LYS:HD3  | 2.14                     | 0.48              |
| 22:d:6005:CLA:HBC2 | 22:d:6005:CLA:CHD  | 2.41                     | 0.48              |
| 10:k:5021:LEU:O    | 10:k:5022:VAL:C    | 2.57                     | 0.48              |
| 14:t:5022:PHE:N    | 14:t:5022:PHE:CD1  | 2.79                     | 0.48              |
| 14:t:5024:ARG:HD2  | 14:t:5024:ARG:C    | 2.38                     | 0.48              |
| 16:v:5114:ILE:O    | 16:v:5114:ILE:CG1  | 2.62                     | 0.48              |
| 16:v:5125:ASP:CG   | 16:v:5126:ILE:HD13 | 2.39                     | 0.48              |
| 1:A:65:GLU:OE1     | 4:D:312:GLU:OE2    | 2.31                     | 0.47              |
| 1:A:119:PHE:CD1    | 23:A:1038:PHO:H122 | 2.50                     | 0.47              |
| 1:A:131:TRP:HD1    | 1:A:141:PRO:HB2    | 1.79                     | 0.47              |
| 2:B:174:LEU:CD2    | 2:B:312:TYR:CZ     | 2.94                     | 0.47              |
| 2:B:457:VAL:CG2    | 4:D:284:ILE:HG23   | 2.44                     | 0.47              |
| 3:C:117:VAL:HG11   | 22:C:1027:CLA:H11  | 1.95                     | 0.47              |
| 3:C:164:HIS:HD1    | 3:C:164:HIS:H      | 1.61                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1033:CLA:H141 | 22:C:1036:CLA:CMD  | 2.44                     | 0.47              |
| 7:H:10:ILE:O       | 7:H:10:ILE:HG22    | 2.14                     | 0.47              |
| 10:K:28:ILE:HA     | 10:K:31:LEU:CD1    | 2.43                     | 0.47              |
| 12:M:8:PHE:O       | 12:M:12:ALA:HB3    | 2.13                     | 0.47              |
| 13:O:151:LEU:HD12  | 13:O:171:GLU:O     | 2.13                     | 0.47              |
| 16:V:114:ILE:O     | 16:V:114:ILE:CG1   | 2.62                     | 0.47              |
| 1:a:5113:GLN:HA    | 1:a:5116:ILE:HG22  | 1.94                     | 0.47              |
| 1:a:5172:MET:HB2   | 1:a:5182:PHE:CD2   | 2.49                     | 0.47              |
| 1:a:5302:PHE:CD1   | 1:a:5302:PHE:N     | 2.82                     | 0.47              |
| 1:a:5340:PRO:HD3   | 15:u:5103:TYR:HE2  | 1.77                     | 0.47              |
| 2:b:5018:ARG:NH1   | 11:l:5004:ASN:HB3  | 2.28                     | 0.47              |
| 2:b:5188:ASP:HB2   | 7:h:5058:VAL:HG22  | 1.96                     | 0.47              |
| 2:b:5297:THR:HB    | 2:b:5300:GLU:H     | 1.78                     | 0.47              |
| 2:b:5326:ARG:HE    | 4:d:5297:ASP:HB2   | 1.78                     | 0.47              |
| 2:b:5461:LEU:O     | 2:b:5464:PHE:HB3   | 2.14                     | 0.47              |
| 22:b:6022:CLA:H203 | 22:b:6022:CLA:C2   | 2.44                     | 0.47              |
| 3:c:5168:LEU:C     | 3:c:5170:ILE:N     | 2.71                     | 0.47              |
| 3:c:5342:MET:HB2   | 3:c:5352:GLY:HA3   | 1.96                     | 0.47              |
| 22:c:6037:CLA:H8   | 22:c:6037:CLA:H142 | 1.96                     | 0.47              |
| 4:d:5250:ASN:CG    | 4:d:5251:ARG:N     | 2.70                     | 0.47              |
| 4:d:5286:VAL:HG13  | 4:d:5287:VAL:N     | 2.28                     | 0.47              |
| 28:d:6062:MGE:H251 | 28:d:6062:MGE:CBB  | 2.44                     | 0.47              |
| 6:f:5041:GLN:HE22  | 9:j:5028:PHE:HA    | 1.74                     | 0.47              |
| 22:k:6034:CLA:H91  | 22:k:6034:CLA:C12  | 2.44                     | 0.47              |
| 13:o:5134:VAL:HG23 | 13:o:5142:ILE:CG2  | 2.44                     | 0.47              |
| 25:t:1046:BCR:H23C | 25:t:1046:BCR:C40  | 2.36                     | 0.47              |
| 16:v:5035:THR:CB   | 16:v:5046:THR:HA   | 2.44                     | 0.47              |
| 1:A:40:THR:HG21    | 1:A:122:GLY:N      | 2.25                     | 0.47              |
| 1:A:101:SER:O      | 1:A:102:LEU:C      | 2.56                     | 0.47              |
| 1:A:214:MET:O      | 1:A:217:SER:HB3    | 2.15                     | 0.47              |
| 1:A:215:HIS:NE2    | 1:A:272:HIS:CE1    | 2.82                     | 0.47              |
| 1:A:303:ASN:N      | 1:A:303:ASN:ND2    | 2.60                     | 0.47              |
| 2:B:49:ASP:OD1     | 2:B:49:ASP:O       | 2.32                     | 0.47              |
| 2:B:122:LEU:HD21   | 7:H:12:ARG:N       | 2.29                     | 0.47              |
| 2:B:355:PHE:HD2    | 2:B:355:PHE:N      | 2.11                     | 0.47              |
| 2:B:452:THR:HG22   | 4:D:291:LEU:HD11   | 1.95                     | 0.47              |
| 2:B:461:LEU:O      | 2:B:464:PHE:HB3    | 2.14                     | 0.47              |
| 22:B:1021:CLA:C11  | 28:B:1060:MGE:H132 | 2.42                     | 0.47              |
| 4:D:37:LEU:CD2     | 4:D:128:ARG:HD3    | 2.27                     | 0.47              |
| 4:D:84:SER:O       | 5:E:69:ARG:HB3     | 2.14                     | 0.47              |
| 4:D:113:PHE:O      | 4:D:114:ILE:C      | 2.57                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:223:PHE:CZ     | 4:D:245:SER:HB2    | 2.48                     | 0.47              |
| 28:D:1062:MGE:H231 | 11:L:26:VAL:CG2    | 2.44                     | 0.47              |
| 11:L:9:PRO:CB      | 12:m:5034:LYS:HE2  | 2.44                     | 0.47              |
| 12:M:9:ILE:O       | 12:M:13:LEU:HB2    | 2.15                     | 0.47              |
| 16:V:101:TYR:HA    | 16:V:104:ASN:O     | 2.14                     | 0.47              |
| 16:V:125:ASP:CG    | 16:V:126:ILE:HD13  | 2.39                     | 0.47              |
| 1:a:5084:PRO:HA    | 1:a:5112:TYR:CG    | 2.48                     | 0.47              |
| 1:a:5119:PHE:CD1   | 23:a:6038:PHO:H122 | 2.50                     | 0.47              |
| 1:a:5161:TYR:CZ    | 1:a:5186:PHE:HE2   | 2.32                     | 0.47              |
| 24:a:6043:PQ9:H311 | 24:a:6043:PQ9:H291 | 1.67                     | 0.47              |
| 2:b:5456:ALA:CA    | 29:b:6058:DGD:HBV1 | 2.42                     | 0.47              |
| 22:b:6022:CLA:O1D  | 22:b:6022:CLA:C1   | 2.62                     | 0.47              |
| 3:c:5039:ASN:HB3   | 22:c:6033:CLA:CBB  | 2.43                     | 0.47              |
| 3:c:5087:ILE:O     | 3:c:5090:PRO:CG    | 2.61                     | 0.47              |
| 3:c:5093:ALA:HB1   | 3:c:5099:VAL:HG21  | 1.96                     | 0.47              |
| 3:c:5377:LEU:HD11  | 3:c:5381:LYS:NZ    | 2.29                     | 0.47              |
| 5:e:5031:PHE:O     | 6:f:5035:GLY:HA3   | 2.13                     | 0.47              |
| 6:f:5020:TRP:HE1   | 31:f:6040:HEM:CHD  | 2.27                     | 0.47              |
| 12:m:5006:LEU:O    | 12:m:5007:GLY:C    | 2.56                     | 0.47              |
| 15:u:5064:ILE:O    | 15:u:5067:LEU:HG   | 2.14                     | 0.47              |
| 1:A:61:ASP:HB2     | 1:A:63:ILE:CD1     | 2.44                     | 0.47              |
| 1:A:172:MET:HB2    | 1:A:182:PHE:CD2    | 2.50                     | 0.47              |
| 1:A:224:ILE:O      | 2:B:481:GLY:HA2    | 2.15                     | 0.47              |
| 1:A:340:PRO:HB3    | 15:U:103:TYR:CD2   | 2.49                     | 0.47              |
| 23:A:1038:PHO:H93  | 23:A:1038:PHO:H62  | 1.68                     | 0.47              |
| 2:B:90:PHE:CZ      | 2:B:98:LEU:HD12    | 2.48                     | 0.47              |
| 2:B:147:GLY:HA2    | 2:B:150:CYS:HB3    | 1.95                     | 0.47              |
| 22:C:1026:CLA:H62  | 22:C:1026:CLA:H2   | 1.63                     | 0.47              |
| 29:C:1056:DGD:O1A  | 29:C:1056:DGD:C5A  | 2.62                     | 0.47              |
| 4:D:261:PHE:H      | 24:D:1042:PQ9:H93  | 1.73                     | 0.47              |
| 7:H:31:MET:HE3     | 7:H:35:MET:SD      | 2.54                     | 0.47              |
| 13:O:52:ALA:O      | 13:O:53:ARG:CB     | 2.62                     | 0.47              |
| 13:O:163:THR:HG23  | 13:O:165:SER:H     | 1.78                     | 0.47              |
| 16:V:90:PRO:HB2    | 16:V:91:PRO:HD2    | 1.96                     | 0.47              |
| 1:a:5096:ILE:HD12  | 22:a:6007:CLA:CMD  | 2.43                     | 0.47              |
| 1:a:5202:VAL:HG23  | 22:a:6003:CLA:HMB2 | 1.95                     | 0.47              |
| 24:a:6043:PQ9:H453 | 24:a:6043:PQ9:H401 | 1.96                     | 0.47              |
| 2:b:5329:PRO:C     | 2:b:5331:ASN:N     | 2.73                     | 0.47              |
| 2:b:5384:ARG:CD    | 15:u:5102:LEU:HD21 | 2.42                     | 0.47              |
| 22:b:6018:CLA:H91  | 22:b:6023:CLA:H3A  | 1.96                     | 0.47              |
| 3:c:5070:PHE:O     | 3:c:5074:HIS:ND1   | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5441:HIS:C     | 3:c:5441:HIS:ND1   | 2.72                     | 0.47              |
| 4:d:5038:PHE:N     | 4:d:5039:PRO:HD2   | 2.30                     | 0.47              |
| 4:d:5193:LEU:HA    | 4:d:5198:MET:HE3   | 1.96                     | 0.47              |
| 16:v:5054:GLU:O    | 16:v:5058:LEU:HB2  | 2.15                     | 0.47              |
| 16:v:5095:ILE:HA   | 16:v:5146:LEU:HD11 | 1.95                     | 0.47              |
| 25:z:6053:BCR:H372 | 25:z:6053:BCR:C36  | 2.14                     | 0.47              |
| 1:A:327:GLY:HA2    | 4:D:328:TRP:CD1    | 2.50                     | 0.47              |
| 2:B:2:GLY:HA2      | 11:L:11:GLU:HB2    | 1.96                     | 0.47              |
| 2:B:57:ARG:C       | 2:B:59:GLY:H       | 2.21                     | 0.47              |
| 2:B:162:PHE:CD1    | 2:B:162:PHE:C      | 2.92                     | 0.47              |
| 2:B:171:PRO:HB3    | 2:B:279:TYR:OH     | 2.15                     | 0.47              |
| 2:B:199:VAL:O      | 2:B:203:ILE:HG22   | 2.15                     | 0.47              |
| 2:B:237:VAL:C      | 22:B:1020:CLA:HMD1 | 2.39                     | 0.47              |
| 2:B:271:THR:H      | 2:B:274:GLN:NE2    | 2.13                     | 0.47              |
| 2:B:271:THR:N      | 2:B:274:GLN:NE2    | 2.62                     | 0.47              |
| 2:B:309:LEU:O      | 2:B:310:ALA:C      | 2.57                     | 0.47              |
| 2:B:397:VAL:HG12   | 2:B:398:THR:N      | 2.29                     | 0.47              |
| 2:B:400:SER:HA     | 2:B:410:THR:HG22   | 1.96                     | 0.47              |
| 22:B:1018:CLA:OBD  | 22:B:1018:CLA:H13  | 2.14                     | 0.47              |
| 3:C:441:HIS:C      | 3:C:441:HIS:ND1    | 2.72                     | 0.47              |
| 3:C:447:ARG:O      | 3:C:450:ALA:HB3    | 2.15                     | 0.47              |
| 4:D:172:SER:OG     | 4:D:177:ALA:HB1    | 2.14                     | 0.47              |
| 4:D:269:PHE:CD1    | 4:D:269:PHE:C      | 2.92                     | 0.47              |
| 4:D:299:ILE:C      | 4:D:301:GLN:N      | 2.72                     | 0.47              |
| 22:D:1008:CLA:HED3 | 22:D:1008:CLA:OBD  | 2.14                     | 0.47              |
| 10:K:28:ILE:HA     | 10:K:31:LEU:CG     | 2.45                     | 0.47              |
| 12:M:17:VAL:N      | 12:M:18:PRO:HD2    | 2.29                     | 0.47              |
| 13:O:45:CYS:N      | 13:O:72:GLN:NE2    | 2.61                     | 0.47              |
| 13:O:128:ASP:O     | 13:O:147:THR:HA    | 2.15                     | 0.47              |
| 20:Z:27:TYR:HE2    | 20:Z:40:ILE:HD13   | 1.79                     | 0.47              |
| 1:a:5063:ILE:CG1   | 1:a:5064:ARG:N     | 2.76                     | 0.47              |
| 1:a:5172:MET:HE2   | 1:a:5179:THR:HA    | 1.95                     | 0.47              |
| 1:a:5244:GLU:HG2   | 4:d:5264:LYS:HZ2   | 1.79                     | 0.47              |
| 22:a:6006:CLA:H143 | 24:a:6043:PQ9:H443 | 1.94                     | 0.47              |
| 2:b:5008:VAL:HG21  | 22:b:6022:CLA:C3D  | 2.44                     | 0.47              |
| 2:b:5026:HIS:HB2   | 22:b:6020:CLA:CMB  | 2.44                     | 0.47              |
| 2:b:5277:SER:C     | 2:b:5279:TYR:N     | 2.71                     | 0.47              |
| 22:b:6023:CLA:H142 | 22:b:6023:CLA:H111 | 1.61                     | 0.47              |
| 4:d:5172:SER:OG    | 4:d:5177:ALA:HB1   | 2.14                     | 0.47              |
| 4:d:5269:PHE:O     | 4:d:5272:LEU:N     | 2.38                     | 0.47              |
| 5:e:5013:ILE:HD12  | 5:e:5016:SER:CB    | 2.44                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:f:5028:VAL:HB    | 6:f:5029:PRO:CD    | 2.38                     | 0.47              |
| 25:k:6051:BCR:C8   | 25:k:6051:BCR:H311 | 2.44                     | 0.47              |
| 12:m:5009:ILE:O    | 12:m:5013:LEU:HB2  | 2.14                     | 0.47              |
| 13:o:5266:TYR:O    | 13:o:5267:ALA:HB2  | 2.15                     | 0.47              |
| 16:v:5154:ASP:O    | 16:v:5156:TRP:N    | 2.47                     | 0.47              |
| 20:z:5037:LYS:CG   | 20:z:5038:GLN:N    | 2.77                     | 0.47              |
| 1:A:41:LEU:CD1     | 1:A:119:PHE:HA     | 2.44                     | 0.47              |
| 1:A:259:ILE:HD12   | 1:A:259:ILE:O      | 2.15                     | 0.47              |
| 2:B:65:PHE:O       | 2:B:67:ALA:N       | 2.48                     | 0.47              |
| 2:B:122:LEU:HD21   | 7:H:11:LEU:HB2     | 1.95                     | 0.47              |
| 2:B:346:PHE:CZ     | 2:B:421:ALA:HA     | 2.49                     | 0.47              |
| 3:C:187:ASP:CB     | 3:C:190:ALA:HB2    | 2.44                     | 0.47              |
| 3:C:191:PRO:O      | 3:C:192:GLY:C      | 2.58                     | 0.47              |
| 3:C:213:LEU:HD21   | 25:C:1054:BCR:H372 | 1.97                     | 0.47              |
| 3:C:428:THR:O      | 3:C:429:SER:C      | 2.56                     | 0.47              |
| 22:C:1029:CLA:HMA3 | 22:C:1029:CLA:HAA2 | 1.58                     | 0.47              |
| 4:D:27:PHE:CD1     | 4:D:28:VAL:HG23    | 2.50                     | 0.47              |
| 4:D:48:TRP:CE2     | 4:D:52:THR:HG21    | 2.49                     | 0.47              |
| 4:D:87:HIS:C       | 4:D:167:TRP:HE1    | 2.20                     | 0.47              |
| 1:a:5288:LEU:HD21  | 3:c:5435:PHE:CD2   | 2.49                     | 0.47              |
| 2:b:5027:THR:HG22  | 2:b:5107:LEU:HD13  | 1.96                     | 0.47              |
| 2:b:5052:LEU:C     | 2:b:5054:PRO:HD3   | 2.39                     | 0.47              |
| 2:b:5271:THR:N     | 2:b:5274:GLN:NE2   | 2.62                     | 0.47              |
| 3:c:5155:ASN:O     | 3:c:5158:THR:CG2   | 2.61                     | 0.47              |
| 3:c:5447:ARG:O     | 3:c:5450:ALA:HB3   | 2.15                     | 0.47              |
| 4:d:5049:LEU:HD13  | 25:d:6050:BCR:C15  | 2.44                     | 0.47              |
| 4:d:5106:GLN:C     | 4:d:5108:GLY:N     | 2.72                     | 0.47              |
| 11:l:5026:VAL:HG12 | 11:l:5027:LEU:HD23 | 1.96                     | 0.47              |
| 15:u:5017:LEU:O    | 15:u:5017:LEU:HD23 | 2.13                     | 0.47              |
| 15:u:5071:GLN:O    | 15:u:5072:LYS:C    | 2.57                     | 0.47              |
| 16:v:5101:TYR:HA   | 16:v:5104:ASN:O    | 2.14                     | 0.47              |
| 22:A:1006:CLA:HAA2 | 29:C:1057:DGD:HBN1 | 1.96                     | 0.47              |
| 2:B:2:GLY:CA       | 11:L:11:GLU:HB2    | 2.44                     | 0.47              |
| 2:B:23:HIS:C       | 2:B:25:MET:H       | 2.21                     | 0.47              |
| 2:B:26:HIS:HB2     | 22:B:1020:CLA:CMB  | 2.44                     | 0.47              |
| 2:B:196:GLY:O      | 2:B:198:VAL:N      | 2.47                     | 0.47              |
| 2:B:326:ARG:HE     | 4:D:297:ASP:HB2    | 1.78                     | 0.47              |
| 22:B:1018:CLA:H91  | 22:B:1023:CLA:H3A  | 1.96                     | 0.47              |
| 3:C:292:PHE:CE1    | 29:C:1055:DGD:HD1  | 2.49                     | 0.47              |
| 3:C:327:ASN:ND2    | 3:C:330:SER:H      | 2.09                     | 0.47              |
| 22:C:1028:CLA:O1D  | 29:C:1056:DGD:HE62 | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1029:CLA:HBD  | 22:C:1029:CLA:HAA1 | 1.97                     | 0.47              |
| 4:D:125:PHE:CD1    | 4:D:125:PHE:C      | 2.92                     | 0.47              |
| 4:D:286:VAL:HG13   | 4:D:287:VAL:N      | 2.28                     | 0.47              |
| 28:D:1062:MGE:CBB  | 28:D:1062:MGE:H251 | 2.43                     | 0.47              |
| 9:J:8:ILE:HD12     | 9:J:8:ILE:N        | 2.29                     | 0.47              |
| 9:J:31:GLY:O       | 9:J:35:GLY:CA      | 2.58                     | 0.47              |
| 15:U:35:PHE:HD1    | 15:U:46:ALA:HB2    | 1.78                     | 0.47              |
| 20:Z:16:SER:HA     | 20:Z:19:MET:HB2    | 1.97                     | 0.47              |
| 1:a:5131:TRP:HD1   | 1:a:5141:PRO:HB2   | 1.79                     | 0.47              |
| 1:a:5316:THR:C     | 1:a:5318:ALA:N     | 2.72                     | 0.47              |
| 2:b:5196:GLY:O     | 2:b:5198:VAL:N     | 2.47                     | 0.47              |
| 2:b:5457:VAL:CG2   | 4:d:5284:ILE:HG23  | 2.44                     | 0.47              |
| 2:b:5461:LEU:O     | 2:b:5464:PHE:N     | 2.37                     | 0.47              |
| 22:b:6009:CLA:CBA  | 22:b:6009:CLA:O2D  | 2.60                     | 0.47              |
| 22:b:6019:CLA:CBB  | 22:b:6021:CLA:HMB3 | 2.43                     | 0.47              |
| 22:b:6022:CLA:C3D  | 22:b:6022:CLA:H201 | 2.44                     | 0.47              |
| 3:c:5164:HIS:H     | 3:c:5164:HIS:HD1   | 1.61                     | 0.47              |
| 3:c:5187:ASP:CB    | 3:c:5190:ALA:HB2   | 2.44                     | 0.47              |
| 3:c:5370:ARG:HD2   | 13:o:5033:TYR:CD1  | 2.50                     | 0.47              |
| 3:c:5403:SER:OG    | 3:c:5405:ASN:HB3   | 2.15                     | 0.47              |
| 22:c:6029:CLA:HBD  | 22:c:6029:CLA:HAA1 | 1.97                     | 0.47              |
| 4:d:5084:SER:O     | 5:e:5069:ARG:HB3   | 2.14                     | 0.47              |
| 4:d:5302:GLU:HA    | 4:d:5305:ALA:HB2   | 1.96                     | 0.47              |
| 25:d:6050:BCR:H24C | 25:d:6050:BCR:H371 | 1.64                     | 0.47              |
| 28:d:6062:MGE:O1B  | 28:d:6062:MGE:C3G  | 2.34                     | 0.47              |
| 5:e:5013:ILE:HD12  | 5:e:5016:SER:HB3   | 1.96                     | 0.47              |
| 6:f:5040:MET:C     | 6:f:5042:PHE:N     | 2.71                     | 0.47              |
| 25:k:6051:BCR:H23C | 25:k:6051:BCR:H392 | 1.95                     | 0.47              |
| 12:m:5009:ILE:O    | 12:m:5013:LEU:HD23 | 2.15                     | 0.47              |
| 12:m:5017:VAL:N    | 12:m:5018:PRO:HD2  | 2.29                     | 0.47              |
| 20:z:5027:TYR:HE2  | 20:z:5040:ILE:HD13 | 1.79                     | 0.47              |
| 1:A:157:VAL:O      | 1:A:158:PHE:HD2    | 1.98                     | 0.47              |
| 1:A:254:TYR:CD1    | 1:A:254:TYR:C      | 2.93                     | 0.47              |
| 1:A:258:LEU:HD21   | 4:D:129:GLN:HG2    | 1.95                     | 0.47              |
| 1:A:290:ILE:HG22   | 1:A:291:SER:H      | 1.78                     | 0.47              |
| 25:A:1044:BCR:HC7  | 8:I:15:PHE:CZ      | 2.50                     | 0.47              |
| 2:B:23:HIS:C       | 2:B:25:MET:N       | 2.73                     | 0.47              |
| 2:B:46:ASP:H       | 2:B:58:GLN:HE22    | 1.63                     | 0.47              |
| 2:B:355:PHE:O      | 2:B:370:LEU:HA     | 2.15                     | 0.47              |
| 22:B:1011:CLA:H202 | 7:H:38:PHE:HE2     | 1.78                     | 0.47              |
| 22:B:1013:CLA:HMB3 | 22:B:1014:CLA:H11  | 1.94                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1018:CLA:HBB2 | 22:H:1017:CLA:H2   | 1.96                     | 0.47              |
| 3:C:83:GLU:CD      | 16:V:129:LYS:HZ1   | 2.23                     | 0.47              |
| 3:C:165:LEU:O      | 3:C:244:CYS:SG     | 2.73                     | 0.47              |
| 3:C:169:GLY:HA2    | 3:C:241:GLY:HA2    | 1.96                     | 0.47              |
| 3:C:362:ARG:HD2    | 3:C:367:GLU:CD     | 2.40                     | 0.47              |
| 3:C:370:ARG:HD2    | 13:O:33:TYR:CD1    | 2.50                     | 0.47              |
| 3:C:377:LEU:HD11   | 3:C:381:LYS:NZ     | 2.29                     | 0.47              |
| 3:C:406:SER:O      | 3:C:418:ASN:HB2    | 2.15                     | 0.47              |
| 25:C:1054:BCR:H371 | 25:C:1054:BCR:H24C | 1.63                     | 0.47              |
| 4:D:38:PHE:N       | 4:D:39:PRO:HD2     | 2.29                     | 0.47              |
| 4:D:64:ALA:O       | 4:D:71:CYS:SG      | 2.72                     | 0.47              |
| 4:D:82:ALA:C       | 4:D:84:SER:N       | 2.73                     | 0.47              |
| 4:D:185:PHE:O      | 4:D:189:HIS:N      | 2.48                     | 0.47              |
| 4:D:193:LEU:HA     | 4:D:198:MET:HE3    | 1.96                     | 0.47              |
| 4:D:214:HIS:CA     | 4:D:217:THR:HG22   | 2.45                     | 0.47              |
| 4:D:301:GLN:HE22   | 4:D:313:THR:HG21   | 1.79                     | 0.47              |
| 24:D:1042:PQ9:C40  | 11:L:30:LEU:HD12   | 2.38                     | 0.47              |
| 6:F:17:THR:O       | 6:F:18:VAL:C       | 2.58                     | 0.47              |
| 6:F:40:MET:C       | 6:F:42:PHE:N       | 2.71                     | 0.47              |
| 8:I:1:MET:C        | 8:I:3:THR:H        | 2.22                     | 0.47              |
| 12:M:34:LYS:HA     | 12:m:5032:GLN:NE2  | 2.30                     | 0.47              |
| 13:O:104:LEU:HD12  | 13:O:104:LEU:C     | 2.40                     | 0.47              |
| 13:O:148:VAL:CG2   | 13:O:151:LEU:HD22  | 2.45                     | 0.47              |
| 13:O:170:GLY:O     | 13:O:222:GLN:HA    | 2.14                     | 0.47              |
| 13:O:215:ARG:HD3   | 13:O:215:ARG:H     | 1.78                     | 0.47              |
| 13:O:241:PHE:HE1   | 13:O:261:ILE:HG22  | 1.79                     | 0.47              |
| 13:O:266:TYR:O     | 13:O:267:ALA:HB2   | 2.15                     | 0.47              |
| 15:U:27:LEU:HD21   | 15:U:82:PHE:CD1    | 2.46                     | 0.47              |
| 15:U:43:PRO:HG3    | 16:V:109:ASP:HA    | 1.97                     | 0.47              |
| 16:V:35:THR:CB     | 16:V:46:THR:HA     | 2.44                     | 0.47              |
| 16:V:83:GLU:O      | 16:V:87:LEU:HG     | 2.15                     | 0.47              |
| 19:N:4:UNK:C       | 19:N:6:UNK:N       | 2.74                     | 0.47              |
| 1:a:5112:TYR:O     | 1:a:5113:GLN:C     | 2.55                     | 0.47              |
| 1:a:5128:GLY:C     | 1:a:5130:GLN:N     | 2.72                     | 0.47              |
| 1:a:5157:VAL:O     | 1:a:5158:PHE:HD2   | 1.98                     | 0.47              |
| 1:a:5214:MET:O     | 1:a:5217:SER:HB3   | 2.15                     | 0.47              |
| 1:a:5255:PHE:O     | 1:a:5256:GLY:C     | 2.56                     | 0.47              |
| 1:a:5259:ILE:HD12  | 1:a:5259:ILE:O     | 2.15                     | 0.47              |
| 22:a:6003:CLA:CED  | 22:a:6003:CLA:CGA  | 2.92                     | 0.47              |
| 2:b:5185:TRP:H     | 2:b:5185:TRP:CD1   | 2.33                     | 0.47              |
| 2:b:5354:LEU:HD21  | 2:b:5378:LYS:HB2   | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5397:VAL:HG12  | 2:b:5398:THR:N     | 2.29                     | 0.47              |
| 3:c:5045:LEU:HA    | 3:c:5045:LEU:HD23  | 1.75                     | 0.47              |
| 3:c:5087:ILE:O     | 3:c:5090:PRO:HG2   | 2.15                     | 0.47              |
| 3:c:5165:LEU:HD21  | 22:c:6030:CLA:HBB1 | 1.96                     | 0.47              |
| 3:c:5176:VAL:HA    | 3:c:5234:VAL:HG23  | 1.95                     | 0.47              |
| 3:c:5237:HIS:O     | 3:c:5238:ILE:C     | 2.58                     | 0.47              |
| 22:c:6027:CLA:C15  | 25:z:6053:BCR:C33  | 2.87                     | 0.47              |
| 22:c:6033:CLA:H141 | 22:c:6036:CLA:CMD  | 2.44                     | 0.47              |
| 29:c:6056:DGD:O1A  | 29:c:6056:DGD:C5A  | 2.62                     | 0.47              |
| 29:c:6056:DGD:HA72 | 29:c:6056:DGD:HAT1 | 1.57                     | 0.47              |
| 4:d:5027:PHE:CD1   | 4:d:5028:VAL:HG23  | 2.50                     | 0.47              |
| 4:d:5125:PHE:CD1   | 4:d:5125:PHE:C     | 2.92                     | 0.47              |
| 4:d:5155:SER:HA    | 4:d:5159:ILE:CB    | 2.44                     | 0.47              |
| 25:h:6049:BCR:H371 | 25:h:6049:BCR:H24C | 1.63                     | 0.47              |
| 8:i:5010:ILE:HD13  | 8:i:5010:ILE:N     | 2.28                     | 0.47              |
| 10:k:5035:LEU:C    | 10:k:5038:VAL:HG23 | 2.38                     | 0.47              |
| 13:o:5128:ASP:O    | 13:o:5147:THR:HA   | 2.15                     | 0.47              |
| 13:o:5170:GLY:O    | 13:o:5222:GLN:HA   | 2.14                     | 0.47              |
| 13:o:5227:VAL:HG11 | 13:o:5230:VAL:CG2  | 2.44                     | 0.47              |
| 16:v:5126:ILE:HD13 | 16:v:5126:ILE:N    | 2.30                     | 0.47              |
| 1:A:199:GLN:C      | 1:A:201:GLY:H      | 2.22                     | 0.47              |
| 1:A:244:GLU:OE2    | 4:D:243:THR:HG22   | 2.15                     | 0.47              |
| 22:A:1007:CLA:C9   | 8:I:16:VAL:HG11    | 2.45                     | 0.47              |
| 2:B:248:ALA:HA     | 22:B:1011:CLA:C5   | 2.45                     | 0.47              |
| 22:B:1020:CLA:H41  | 22:B:1020:CLA:C8   | 2.45                     | 0.47              |
| 3:C:75:PHE:HD1     | 3:C:86:LEU:HD11    | 1.78                     | 0.47              |
| 3:C:403:SER:OG     | 3:C:405:ASN:HB3    | 2.15                     | 0.47              |
| 3:C:440:GLY:C      | 3:C:442:LEU:N      | 2.72                     | 0.47              |
| 3:C:461:ARG:HG2    | 4:D:223:PHE:CD2    | 2.50                     | 0.47              |
| 29:C:1055:DGD:C6A  | 29:C:1055:DGD:CAA  | 2.85                     | 0.47              |
| 4:D:120:PHE:O      | 4:D:121:GLY:C      | 2.55                     | 0.47              |
| 4:D:269:PHE:O      | 4:D:272:LEU:HB3    | 2.15                     | 0.47              |
| 5:E:13:ILE:HD12    | 5:E:16:SER:HB3     | 1.96                     | 0.47              |
| 13:O:134:VAL:HG23  | 13:O:142:ILE:CG2   | 2.44                     | 0.47              |
| 15:U:21:TYR:HE2    | 15:U:30:THR:HG1    | 1.60                     | 0.47              |
| 15:U:64:ILE:O      | 15:U:67:LEU:HG     | 2.14                     | 0.47              |
| 15:U:78:ASN:C      | 15:U:82:PHE:HE2    | 2.23                     | 0.47              |
| 1:a:5061:ASP:HB2   | 1:a:5063:ILE:HD13  | 1.96                     | 0.47              |
| 1:a:5284:TRP:O     | 1:a:5285:PHE:C     | 2.56                     | 0.47              |
| 1:a:5340:PRO:HB3   | 15:u:5103:TYR:CD2  | 2.49                     | 0.47              |
| 25:a:6044:BCR:HC7  | 8:i:5015:PHE:CZ    | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5023:HIS:C     | 2:b:5025:MET:H     | 2.21                     | 0.47              |
| 2:b:5042:LEU:HD21  | 2:b:5093:PHE:HB3   | 1.97                     | 0.47              |
| 2:b:5168:VAL:CG1   | 2:b:5169:SER:N     | 2.76                     | 0.47              |
| 2:b:5237:VAL:C     | 22:b:6020:CLA:HMD1 | 2.39                     | 0.47              |
| 22:b:6016:CLA:C17  | 22:d:6008:CLA:HMA1 | 2.34                     | 0.47              |
| 3:c:5043:ILE:HG13  | 22:c:6033:CLA:HAC2 | 1.96                     | 0.47              |
| 3:c:5157:MET:HB3   | 22:c:6031:CLA:HBC1 | 1.95                     | 0.47              |
| 3:c:5191:PRO:O     | 3:c:5192:GLY:C     | 2.58                     | 0.47              |
| 3:c:5213:LEU:HD21  | 25:c:6054:BCR:H372 | 1.97                     | 0.47              |
| 3:c:5305:THR:HG23  | 3:c:5308:GLU:H     | 1.79                     | 0.47              |
| 3:c:5362:ARG:HD2   | 3:c:5367:GLU:CD    | 2.40                     | 0.47              |
| 29:c:6056:DGD:HBf1 | 29:c:6056:DGD:HB81 | 1.95                     | 0.47              |
| 4:d:5064:ALA:O     | 4:d:5071:CYS:SG    | 2.72                     | 0.47              |
| 4:d:5309:PRO:O     | 13:o:5185:PRO:HD2  | 2.15                     | 0.47              |
| 6:f:5029:PRO:O     | 6:f:5030:THR:C     | 2.58                     | 0.47              |
| 7:h:5031:MET:HE3   | 7:h:5035:MET:SD    | 2.54                     | 0.47              |
| 9:j:5015:THR:CG2   | 10:k:5038:VAL:HG13 | 2.45                     | 0.47              |
| 10:k:5032:PHE:CD1  | 25:k:6052:BCR:H372 | 2.50                     | 0.47              |
| 13:o:5241:PHE:HE1  | 13:o:5261:ILE:HG22 | 1.79                     | 0.47              |
| 25:t:1046:BCR:H371 | 25:t:1046:BCR:H24C | 1.61                     | 0.47              |
| 15:u:5046:ALA:O    | 15:u:5050:VAL:HG23 | 2.15                     | 0.47              |
| 17:x:5019:PHE:O    | 17:x:5022:GLY:N    | 2.48                     | 0.47              |
| 17:x:5039:ALA:O    | 17:x:5043:ILE:HD13 | 2.15                     | 0.47              |
| 19:n:5004:UNK:C    | 19:n:5006:UNK:N    | 2.74                     | 0.47              |
| 1:A:96:ILE:HD12    | 22:A:1007:CLA:HMD1 | 1.96                     | 0.47              |
| 1:A:210:LEU:C      | 1:A:210:LEU:CD2    | 2.84                     | 0.47              |
| 3:C:161:LEU:HD23   | 3:C:161:LEU:C      | 2.40                     | 0.47              |
| 3:C:273:SER:O      | 3:C:274:TYR:O      | 2.33                     | 0.47              |
| 3:C:348:GLU:OE2    | 3:C:349:ILE:CG1    | 2.63                     | 0.47              |
| 4:D:262:SER:O      | 4:D:263:ASN:CB     | 2.61                     | 0.47              |
| 4:D:307:GLU:O      | 4:D:308:ASP:C      | 2.58                     | 0.47              |
| 4:D:309:PRO:O      | 13:O:185:PRO:HD2   | 2.15                     | 0.47              |
| 5:E:26:THR:HG22    | 19:N:14:UNK:O      | 2.15                     | 0.47              |
| 5:E:79:PHE:C       | 5:E:83:LEU:HD13    | 2.38                     | 0.47              |
| 22:K:1034:CLA:CGA  | 22:K:1034:CLA:O2D  | 2.63                     | 0.47              |
| 15:U:71:GLN:O      | 15:U:72:LYS:C      | 2.57                     | 0.47              |
| 1:a:5040:THR:HG21  | 1:a:5122:GLY:N     | 2.25                     | 0.47              |
| 1:a:5156:ALA:HB1   | 1:a:5290:ILE:HG22  | 1.97                     | 0.47              |
| 1:a:5223:LEU:HD21  | 4:d:5265:ARG:CD    | 2.44                     | 0.47              |
| 1:a:5327:GLY:HA2   | 4:d:5328:TRP:CD1   | 2.50                     | 0.47              |
| 2:b:5338:GLN:HA    | 2:b:5338:GLN:NE2   | 2.16                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5355:PHE:CD2   | 2:b:5355:PHE:N     | 2.81                     | 0.47              |
| 2:b:5392:PHE:CE2   | 2:b:5417:VAL:HG12  | 2.50                     | 0.47              |
| 3:c:5284:PHE:CE1   | 3:c:5431:PHE:CD2   | 3.03                     | 0.47              |
| 22:c:6033:CLA:HBD  | 22:c:6033:CLA:HAA2 | 1.97                     | 0.47              |
| 4:d:5312:GLU:HG3   | 13:o:5185:PRO:HB3  | 1.97                     | 0.47              |
| 8:i:5004:LEU:O     | 8:i:5007:THR:OG1   | 2.26                     | 0.47              |
| 20:z:5020:VAL:O    | 20:z:5021:ILE:C    | 2.58                     | 0.47              |
| 1:A:205:VAL:CB     | 1:A:279:ARG:NH2    | 2.78                     | 0.47              |
| 1:A:209:ALA:HB2    | 4:D:204:VAL:O      | 2.15                     | 0.47              |
| 1:A:223:LEU:HD21   | 4:D:265:ARG:CD     | 2.44                     | 0.47              |
| 1:A:265:PHE:HD1    | 1:A:271:LEU:HA     | 1.79                     | 0.47              |
| 2:B:22:ALA:O       | 2:B:25:MET:N       | 2.41                     | 0.47              |
| 2:B:347:ARG:HB2    | 2:B:398:THR:HG23   | 1.96                     | 0.47              |
| 2:B:360:PRO:O      | 2:B:362:PHE:N      | 2.48                     | 0.47              |
| 2:B:474:LEU:C      | 2:B:475:PHE:HD2    | 2.23                     | 0.47              |
| 22:B:1018:CLA:CBB  | 22:H:1017:CLA:O1A  | 2.63                     | 0.47              |
| 25:B:1047:BCR:C12  | 25:B:1047:BCR:C34  | 2.88                     | 0.47              |
| 3:C:312:ALA:HA     | 3:C:365:TRP:CH2    | 2.50                     | 0.47              |
| 29:C:1055:DGD:HBG2 | 29:C:1055:DGD:CEB  | 2.27                     | 0.47              |
| 4:D:297:ASP:OD1    | 4:D:298:PHE:N      | 2.27                     | 0.47              |
| 4:D:312:GLU:HG3    | 13:O:185:PRO:HB3   | 1.97                     | 0.47              |
| 15:U:51:LYS:O      | 15:U:52:ASN:HB2    | 2.15                     | 0.47              |
| 15:U:68:THR:HG23   | 15:U:70:ARG:N      | 2.22                     | 0.47              |
| 16:V:92:ARG:CG     | 16:V:92:ARG:NH1    | 2.67                     | 0.47              |
| 1:a:5076:ASN:ND2   | 11:l:5033:SER:CB   | 2.67                     | 0.47              |
| 1:a:5183:MET:C     | 22:a:6003:CLA:CBC  | 2.88                     | 0.47              |
| 1:a:5204:GLY:O     | 1:a:5207:GLY:N     | 2.48                     | 0.47              |
| 1:a:5210:LEU:HD22  | 1:a:5211:PHE:CD2   | 2.50                     | 0.47              |
| 1:a:5244:GLU:OE2   | 4:d:5243:THR:HG22  | 2.15                     | 0.47              |
| 2:b:5049:ASP:OD1   | 2:b:5049:ASP:O     | 2.32                     | 0.47              |
| 2:b:5108:PHE:C     | 2:b:5111:ALA:HB3   | 2.38                     | 0.47              |
| 2:b:5199:VAL:O     | 2:b:5203:ILE:HG22  | 2.15                     | 0.47              |
| 2:b:5329:PRO:C     | 2:b:5331:ASN:H     | 2.23                     | 0.47              |
| 2:b:5346:PHE:CZ    | 2:b:5421:ALA:HA    | 2.49                     | 0.47              |
| 3:c:5337:LEU:HD13  | 3:c:5342:MET:HE2   | 1.97                     | 0.47              |
| 22:c:6028:CLA:H93  | 29:c:6056:DGD:HB91 | 1.97                     | 0.47              |
| 22:c:6031:CLA:H142 | 25:c:6054:BCR:H362 | 1.91                     | 0.47              |
| 22:d:6005:CLA:H202 | 22:d:6005:CLA:C15  | 2.42                     | 0.47              |
| 9:j:5038:SER:O     | 9:j:5039:SER:OG    | 2.31                     | 0.47              |
| 15:u:5045:LEU:HD21 | 15:u:5075:LEU:HD11 | 1.92                     | 0.47              |
| 15:u:5068:THR:HG23 | 15:u:5070:ARG:N    | 2.22                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:v:5098:LEU:HB3  | 16:v:5102:MET:HE2  | 1.97                     | 0.47              |
| 1:A:76:ASN:HD22    | 11:L:33:SER:HB3    | 1.75                     | 0.46              |
| 1:A:197:PHE:HE1    | 1:A:285:PHE:CD2    | 2.23                     | 0.46              |
| 2:B:33:TRP:O       | 2:B:36:SER:HB2     | 2.15                     | 0.46              |
| 2:B:115:TRP:CB     | 27:B:1067:IOD:I    | 3.33                     | 0.46              |
| 2:B:149:LEU:HD13   | 22:B:1012:CLA:H201 | 1.97                     | 0.46              |
| 3:C:42:LEU:CD1     | 3:C:49:LEU:HD12    | 2.37                     | 0.46              |
| 3:C:43:ILE:HG13    | 22:C:1033:CLA:HAC2 | 1.96                     | 0.46              |
| 3:C:307:PRO:HB3    | 3:C:358:PHE:CG     | 2.50                     | 0.46              |
| 22:C:1030:CLA:CMB  | 22:C:1031:CLA:C4B  | 2.85                     | 0.46              |
| 4:D:319:LEU:O      | 4:D:319:LEU:HD23   | 2.15                     | 0.46              |
| 5:E:27:ILE:HG13    | 31:F:1040:HEM:CMB  | 2.46                     | 0.46              |
| 11:L:26:VAL:HG12   | 11:L:27:LEU:HD23   | 1.96                     | 0.46              |
| 12:M:9:ILE:O       | 12:M:13:LEU:HD23   | 2.15                     | 0.46              |
| 13:O:145:LEU:O     | 13:O:146:PHE:C     | 2.59                     | 0.46              |
| 16:V:126:ILE:HD13  | 16:V:126:ILE:N     | 2.30                     | 0.46              |
| 17:X:19:PHE:O      | 17:X:22:GLY:N      | 2.48                     | 0.46              |
| 20:Z:37:LYS:CG     | 20:Z:38:GLN:N      | 2.77                     | 0.46              |
| 1:a:5305:SER:HA    | 9:j:5039:SER:HB3   | 1.97                     | 0.46              |
| 1:a:5323:ARG:C     | 1:a:5325:ASN:N     | 2.73                     | 0.46              |
| 2:b:5023:HIS:C     | 2:b:5025:MET:N     | 2.73                     | 0.46              |
| 2:b:5098:LEU:C     | 2:b:5098:LEU:CD1   | 2.87                     | 0.46              |
| 2:b:5360:PRO:O     | 2:b:5362:PHE:N     | 2.48                     | 0.46              |
| 3:c:5079:LYS:HB3   | 3:c:5084:GLN:HE21  | 1.75                     | 0.46              |
| 3:c:5083:GLU:CD    | 16:v:5129:LYS:HZ1  | 2.23                     | 0.46              |
| 3:c:5161:LEU:HD23  | 3:c:5161:LEU:C     | 2.40                     | 0.46              |
| 3:c:5223:TRP:HD1   | 3:c:5224:ILE:N     | 2.13                     | 0.46              |
| 3:c:5307:PRO:HB3   | 3:c:5358:PHE:CG    | 2.50                     | 0.46              |
| 3:c:5318:LEU:HA    | 3:c:5340:TYR:HD1   | 1.80                     | 0.46              |
| 3:c:5406:SER:O     | 3:c:5418:ASN:HB2   | 2.15                     | 0.46              |
| 3:c:5440:GLY:C     | 3:c:5442:LEU:N     | 2.72                     | 0.46              |
| 22:c:6032:CLA:H121 | 10:k:5033:PHE:CZ   | 2.50                     | 0.46              |
| 4:d:5048:TRP:CE2   | 4:d:5052:THR:HG21  | 2.49                     | 0.46              |
| 4:d:5183:LEU:H     | 4:d:5183:LEU:CD2   | 2.18                     | 0.46              |
| 4:d:5312:GLU:CG    | 13:o:5185:PRO:HB3  | 2.45                     | 0.46              |
| 7:h:5010:ILE:HG22  | 7:h:5010:ILE:O     | 2.14                     | 0.46              |
| 7:h:5017:GLU:CB    | 7:h:5020:LYS:HD3   | 2.45                     | 0.46              |
| 8:i:5004:LEU:O     | 8:i:5005:LYS:C     | 2.58                     | 0.46              |
| 22:k:6034:CLA:CGA  | 22:k:6034:CLA:O2D  | 2.63                     | 0.46              |
| 14:t:5011:ALA:HB3  | 25:t:1046:BCR:H362 | 1.96                     | 0.46              |
| 14:t:5018:PHE:HD2  | 14:t:5019:PHE:CE2  | 2.34                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:u:5035:PHE:HE1  | 15:u:5049:ILE:HB   | 1.80                     | 0.46              |
| 15:u:5055:TYR:N    | 15:u:5055:TYR:CD1  | 2.82                     | 0.46              |
| 18:y:5043:ARG:CD   | 20:z:5031:GLN:HE21 | 2.28                     | 0.46              |
| 1:A:63:ILE:HG21    | 3:C:335:THR:HB     | 1.98                     | 0.46              |
| 1:A:193:LEU:O      | 1:A:193:LEU:HD23   | 2.15                     | 0.46              |
| 1:A:219:VAL:HG11   | 4:D:268:HIS:CB     | 2.45                     | 0.46              |
| 1:A:224:ILE:CG2    | 1:A:225:ARG:N      | 2.77                     | 0.46              |
| 1:A:279:ARG:NH2    | 1:A:283:VAL:HG22   | 2.30                     | 0.46              |
| 2:B:25:MET:O       | 2:B:26:HIS:C       | 2.56                     | 0.46              |
| 2:B:70:GLY:HA2     | 2:B:178:VAL:HG21   | 1.96                     | 0.46              |
| 2:B:329:PRO:C      | 2:B:331:ASN:N      | 2.73                     | 0.46              |
| 2:B:354:LEU:HD21   | 2:B:378:LYS:HB2    | 1.97                     | 0.46              |
| 2:B:360:PRO:HG2    | 2:B:363:PHE:CD2    | 2.50                     | 0.46              |
| 22:B:1018:CLA:H2   | 22:B:1018:CLA:H111 | 1.97                     | 0.46              |
| 3:C:160:ILE:O      | 3:C:161:LEU:C      | 2.57                     | 0.46              |
| 3:C:171:GLY:CA     | 22:C:1025:CLA:CBC  | 2.93                     | 0.46              |
| 4:D:57:SER:HB3     | 4:D:65:SER:OG      | 2.15                     | 0.46              |
| 4:D:103:ARG:O      | 4:D:106:GLN:N      | 2.48                     | 0.46              |
| 4:D:226:GLY:CA     | 4:D:234:ALA:CB     | 2.92                     | 0.46              |
| 22:D:1005:CLA:H41  | 22:D:1005:CLA:H61  | 1.58                     | 0.46              |
| 25:D:1050:BCR:H371 | 25:D:1050:BCR:H24C | 1.64                     | 0.46              |
| 11:L:26:VAL:O      | 11:L:27:LEU:C      | 2.58                     | 0.46              |
| 13:O:76:PHE:CE2    | 13:O:132:VAL:HG21  | 2.45                     | 0.46              |
| 13:O:184:ASP:CG    | 13:O:188:ARG:NH1   | 2.74                     | 0.46              |
| 16:V:88:ALA:HA     | 16:V:108:TYR:CD2   | 2.48                     | 0.46              |
| 1:a:5104:GLU:HG3   | 13:o:5097:VAL:O    | 2.15                     | 0.46              |
| 1:a:5193:LEU:O     | 1:a:5193:LEU:HD23  | 2.15                     | 0.46              |
| 1:a:5210:LEU:HA    | 23:d:6039:PHO:CAC  | 2.43                     | 0.46              |
| 2:b:5347:ARG:HB2   | 2:b:5398:THR:HG23  | 1.96                     | 0.46              |
| 22:b:6023:CLA:H2   | 22:b:6023:CLA:H61  | 1.47                     | 0.46              |
| 3:c:5276:LEU:C     | 3:c:5276:LEU:CD2   | 2.88                     | 0.46              |
| 3:c:5461:ARG:HG2   | 4:d:5223:PHE:CD2   | 2.50                     | 0.46              |
| 22:c:6030:CLA:HAA1 | 22:c:6030:CLA:HBD  | 1.95                     | 0.46              |
| 4:d:5082:ALA:C     | 4:d:5084:SER:N     | 2.73                     | 0.46              |
| 4:d:5315:TYR:O     | 4:d:5319:LEU:HB2   | 2.16                     | 0.46              |
| 4:d:5348:ARG:HH21  | 4:d:5352:LEU:C     | 2.23                     | 0.46              |
| 5:e:5037:PHE:CE1   | 5:e:5043:ALA:HA    | 2.50                     | 0.46              |
| 5:e:5073:LYS:O     | 5:e:5076:VAL:CG2   | 2.54                     | 0.46              |
| 10:k:5032:PHE:O    | 10:k:5035:LEU:N    | 2.47                     | 0.46              |
| 14:t:5011:ALA:O    | 14:t:5012:CYS:C    | 2.56                     | 0.46              |
| 16:v:5090:PRO:HB2  | 16:v:5091:PRO:HD2  | 1.96                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:v:5096:GLU:O    | 16:v:5099:VAL:N    | 2.39                     | 0.46              |
| 1:A:104:GLU:HG3    | 13:O:97:VAL:O      | 2.16                     | 0.46              |
| 1:A:147:TYR:HE2    | 23:A:1038:PHO:HAA1 | 1.80                     | 0.46              |
| 1:A:156:ALA:HB1    | 1:A:290:ILE:HG22   | 1.97                     | 0.46              |
| 1:A:339:PHE:CB     | 1:A:340:PRO:HD2    | 2.41                     | 0.46              |
| 2:B:5:TRP:HA       | 2:B:8:VAL:HG11     | 1.88                     | 0.46              |
| 2:B:37:MET:O       | 2:B:40:TYR:HB3     | 2.14                     | 0.46              |
| 2:B:75:TRP:H       | 2:B:75:TRP:HD1     | 1.63                     | 0.46              |
| 2:B:188:ASP:HB2    | 7:H:58:VAL:HG22    | 1.96                     | 0.46              |
| 2:B:220:ARG:CD     | 7:H:20:LYS:O       | 2.58                     | 0.46              |
| 2:B:265:ILE:H      | 2:B:265:ILE:CD1    | 2.05                     | 0.46              |
| 2:B:377:VAL:HG11   | 4:D:342:PRO:HG2    | 1.97                     | 0.46              |
| 2:B:392:PHE:CE2    | 2:B:417:VAL:HG12   | 2.50                     | 0.46              |
| 3:C:42:LEU:HG      | 3:C:42:LEU:O       | 2.16                     | 0.46              |
| 3:C:337:LEU:HD13   | 3:C:342:MET:HE2    | 1.97                     | 0.46              |
| 22:D:1008:CLA:HMA3 | 22:D:1008:CLA:HAA2 | 1.82                     | 0.46              |
| 5:E:8:ARG:HB2      | 6:F:13:TYR:HB3     | 1.98                     | 0.46              |
| 6:F:24:HIS:C       | 6:F:26:LEU:N       | 2.73                     | 0.46              |
| 6:F:41:GLN:HG3     | 9:J:27:LEU:HD21    | 1.96                     | 0.46              |
| 8:I:4:LEU:O        | 8:I:5:LYS:C        | 2.58                     | 0.46              |
| 10:K:19:ASP:O      | 10:K:23:ASP:OD1    | 2.33                     | 0.46              |
| 11:L:13:ASN:O      | 11:L:15:THR:N      | 2.48                     | 0.46              |
| 12:M:8:PHE:CE2     | 14:T:1:MET:HG3     | 2.50                     | 0.46              |
| 25:T:6046:BCR:C34  | 25:b:6047:BCR:H272 | 2.46                     | 0.46              |
| 16:V:54:GLU:O      | 16:V:58:LEU:HB2    | 2.15                     | 0.46              |
| 16:V:90:PRO:O      | 16:V:91:PRO:C      | 2.55                     | 0.46              |
| 1:a:5254:TYR:CD1   | 1:a:5254:TYR:C     | 2.93                     | 0.46              |
| 1:a:5330:VAL:CG1   | 4:d:5348:ARG:HG2   | 2.45                     | 0.46              |
| 2:b:5065:PHE:O     | 2:b:5067:ALA:N     | 2.48                     | 0.46              |
| 2:b:5075:TRP:H     | 2:b:5075:TRP:HD1   | 1.63                     | 0.46              |
| 22:b:6011:CLA:H92  | 22:b:6011:CLA:CBB  | 2.44                     | 0.46              |
| 22:b:6016:CLA:H92  | 22:h:6017:CLA:H111 | 1.98                     | 0.46              |
| 22:b:6021:CLA:CED  | 22:b:6021:CLA:HMA3 | 2.46                     | 0.46              |
| 3:c:5334:PRO:HG2   | 4:d:5350:ASN:ND2   | 2.31                     | 0.46              |
| 22:c:6037:CLA:H111 | 22:c:6037:CLA:H72  | 1.60                     | 0.46              |
| 4:d:5126:MET:O     | 4:d:5129:GLN:HB2   | 2.16                     | 0.46              |
| 4:d:5287:VAL:O     | 4:d:5290:ALA:HB3   | 2.16                     | 0.46              |
| 4:d:5326:ARG:O     | 4:d:5328:TRP:N     | 2.49                     | 0.46              |
| 5:e:5079:PHE:C     | 5:e:5081:GLU:N     | 2.72                     | 0.46              |
| 9:j:5025:VAL:HG12  | 9:j:5026:GLY:N     | 2.29                     | 0.46              |
| 13:o:5080:GLU:N    | 13:o:5090:GLU:O    | 2.48                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5148:VAL:CG2  | 13:o:5151:LEU:HD22 | 2.45                     | 0.46              |
| 15:u:5074:ILE:O    | 15:u:5075:LEU:C    | 2.58                     | 0.46              |
| 15:u:5078:ASN:C    | 15:u:5082:PHE:HE2  | 2.23                     | 0.46              |
| 1:A:107:TYR:CD2    | 13:O:97:VAL:CG1    | 2.99                     | 0.46              |
| 1:A:183:MET:C      | 22:A:1003:CLA:CBC  | 2.88                     | 0.46              |
| 1:A:193:LEU:HD22   | 4:D:179:PHE:CE2    | 2.50                     | 0.46              |
| 1:A:210:LEU:HA     | 23:D:1039:PHO:CAC  | 2.43                     | 0.46              |
| 1:A:278:TRP:CH2    | 29:C:1057:DGD:HAV2 | 2.51                     | 0.46              |
| 22:B:1023:CLA:H151 | 22:B:1024:CLA:NA   | 2.31                     | 0.46              |
| 3:C:56:HIS:HE1     | 22:C:1033:CLA:HMA1 | 1.81                     | 0.46              |
| 3:C:165:LEU:HD21   | 22:C:1030:CLA:HBB1 | 1.96                     | 0.46              |
| 4:D:53:THR:CG2     | 4:D:67:TYR:CD2     | 2.99                     | 0.46              |
| 4:D:199:MET:HE3    | 24:D:1042:PQ9:H352 | 1.96                     | 0.46              |
| 4:D:269:PHE:C      | 4:D:271:MET:N      | 2.72                     | 0.46              |
| 13:O:163:THR:C     | 13:O:165:SER:N     | 2.72                     | 0.46              |
| 15:U:46:ALA:O      | 15:U:50:VAL:HG23   | 2.15                     | 0.46              |
| 1:a:5096:ILE:HD12  | 22:a:6007:CLA:HMD1 | 1.96                     | 0.46              |
| 1:a:5147:TYR:HE2   | 23:a:6038:PHO:HAA1 | 1.80                     | 0.46              |
| 1:a:5199:GLN:C     | 1:a:5201:GLY:H     | 2.22                     | 0.46              |
| 2:b:5002:GLY:CA    | 11:l:5011:GLU:HB2  | 2.44                     | 0.46              |
| 2:b:5037:MET:O     | 2:b:5040:TYR:HB3   | 2.14                     | 0.46              |
| 2:b:5174:LEU:CD2   | 2:b:5265:ILE:HB    | 2.46                     | 0.46              |
| 2:b:5432:PHE:CE2   | 13:o:5202:GLN:NE2  | 2.83                     | 0.46              |
| 22:b:6018:CLA:H142 | 22:b:6018:CLA:H112 | 1.64                     | 0.46              |
| 22:b:6018:CLA:CBB  | 22:h:6017:CLA:O1A  | 2.63                     | 0.46              |
| 22:b:6022:CLA:H3A  | 22:b:6022:CLA:HBA2 | 1.68                     | 0.46              |
| 3:c:5056:HIS:HE1   | 22:c:6033:CLA:HMA1 | 1.80                     | 0.46              |
| 3:c:5131:TYR:CG    | 3:c:5132:HIS:N     | 2.83                     | 0.46              |
| 3:c:5312:ALA:HA    | 3:c:5365:TRP:CH2   | 2.50                     | 0.46              |
| 3:c:5316:THR:CG2   | 16:v:5074:THR:HG23 | 2.45                     | 0.46              |
| 4:d:5016:ASP:O     | 4:d:5020:ASP:N     | 2.45                     | 0.46              |
| 4:d:5185:PHE:O     | 4:d:5189:HIS:N     | 2.48                     | 0.46              |
| 4:d:5267:LEU:O     | 4:d:5268:HIS:C     | 2.58                     | 0.46              |
| 4:d:5269:PHE:O     | 4:d:5272:LEU:HB3   | 2.15                     | 0.46              |
| 6:f:5017:THR:O     | 6:f:5018:VAL:C     | 2.58                     | 0.46              |
| 6:f:5019:ARG:HH21  | 6:f:5020:TRP:CD1   | 2.34                     | 0.46              |
| 10:k:5035:LEU:C    | 10:k:5037:PHE:N    | 2.72                     | 0.46              |
| 13:o:5184:ASP:CG   | 13:o:5188:ARG:NH1  | 2.73                     | 0.46              |
| 18:y:5039:LEU:HD21 | 20:z:5025:VAL:HA   | 1.98                     | 0.46              |
| 2:B:237:VAL:C      | 22:B:1020:CLA:CMD  | 2.89                     | 0.46              |
| 2:B:250:PHE:HB3    | 29:B:1058:DGD:HB82 | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:329:PRO:C      | 2:B:331:ASN:H      | 2.23                     | 0.46              |
| 2:B:432:PHE:CE2    | 13:O:202:GLN:NE2   | 2.83                     | 0.46              |
| 22:B:1012:CLA:H12  | 22:B:1013:CLA:C4   | 2.37                     | 0.46              |
| 3:C:63:TRP:NE1     | 22:C:1028:CLA:HMC1 | 2.31                     | 0.46              |
| 3:C:259:TRP:CE3    | 3:C:260:ALA:N      | 2.84                     | 0.46              |
| 3:C:277:GLY:HA3    | 3:C:441:HIS:HD2    | 1.81                     | 0.46              |
| 3:C:369:LEU:HD11   | 3:C:384:ILE:CG1    | 2.46                     | 0.46              |
| 3:C:472:LEU:O      | 3:C:473:ASP:CB     | 2.58                     | 0.46              |
| 22:C:1032:CLA:H12  | 22:C:1035:CLA:C3C  | 2.44                     | 0.46              |
| 22:C:1036:CLA:H102 | 22:C:1036:CLA:H13  | 1.50                     | 0.46              |
| 4:D:287:VAL:O      | 4:D:290:ALA:HB3    | 2.16                     | 0.46              |
| 22:H:1017:CLA:HBB1 | 25:H:1049:BCR:C32  | 2.42                     | 0.46              |
| 9:J:25:VAL:HG12    | 9:J:26:GLY:N       | 2.29                     | 0.46              |
| 13:O:184:ASP:OD2   | 13:O:188:ARG:HB2   | 2.15                     | 0.46              |
| 14:T:11:ALA:C      | 14:T:13:ILE:N      | 2.74                     | 0.46              |
| 16:V:105:PRO:HD3   | 16:V:120:SER:CB    | 2.46                     | 0.46              |
| 17:X:13:THR:O      | 17:X:16:LEU:N      | 2.49                     | 0.46              |
| 1:a:5063:ILE:HG21  | 3:c:5335:THR:HB    | 1.98                     | 0.46              |
| 1:a:5224:ILE:O     | 2:b:5481:GLY:HA2   | 2.15                     | 0.46              |
| 2:b:5149:LEU:HD13  | 22:b:6012:CLA:H201 | 1.97                     | 0.46              |
| 2:b:5355:PHE:O     | 2:b:5370:LEU:HA    | 2.15                     | 0.46              |
| 3:c:5036:TRP:O     | 22:c:6032:CLA:H42  | 2.16                     | 0.46              |
| 3:c:5079:LYS:HB3   | 3:c:5084:GLN:CD    | 2.39                     | 0.46              |
| 4:d:5029:PHE:CD2   | 4:d:5029:PHE:C     | 2.93                     | 0.46              |
| 23:d:6039:PHO:HHB  | 22:d:6004:CLA:H121 | 1.98                     | 0.46              |
| 6:f:5041:GLN:HG3   | 9:j:5027:LEU:HD21  | 1.96                     | 0.46              |
| 15:u:5044:THR:O    | 15:u:5047:LYS:N    | 2.49                     | 0.46              |
| 17:x:5013:THR:O    | 17:x:5016:LEU:N    | 2.49                     | 0.46              |
| 17:x:5033:THR:HG22 | 17:x:5034:PHE:N    | 2.31                     | 0.46              |
| 18:y:5028:ILE:CG1  | 18:y:5029:GLY:N    | 2.78                     | 0.46              |
| 1:A:32:TRP:HA      | 1:A:32:TRP:CE3     | 2.50                     | 0.46              |
| 1:A:330:VAL:CG1    | 4:D:348:ARG:HG2    | 2.45                     | 0.46              |
| 2:B:149:LEU:CB     | 22:B:1011:CLA:HBC1 | 2.46                     | 0.46              |
| 2:B:172:TYR:CG     | 2:B:173:GLY:N      | 2.84                     | 0.46              |
| 2:B:224:ARG:HG2    | 7:H:25:TRP:CD1     | 2.51                     | 0.46              |
| 22:B:1021:CLA:CED  | 22:B:1021:CLA:HMA3 | 2.46                     | 0.46              |
| 22:B:1022:CLA:C4   | 22:B:1022:CLA:O2A  | 2.64                     | 0.46              |
| 3:C:87:ILE:O       | 3:C:90:PRO:HG2     | 2.15                     | 0.46              |
| 3:C:100:GLY:O      | 3:C:101:PRO:C      | 2.58                     | 0.46              |
| 3:C:143:TYR:O      | 3:C:144:SER:C      | 2.59                     | 0.46              |
| 3:C:315:MET:HE3    | 3:C:315:MET:CA     | 2.37                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:316:THR:CG2    | 16:V:74:THR:HG23   | 2.45                     | 0.46              |
| 3:C:376:ASP:OD1    | 3:C:378:ASN:HB2    | 2.15                     | 0.46              |
| 22:C:1035:CLA:CMB  | 25:C:1052:BCR:H272 | 2.45                     | 0.46              |
| 29:C:1056:DGD:O1A  | 29:C:1056:DGD:HA52 | 2.16                     | 0.46              |
| 4:D:210:LEU:HD12   | 4:D:210:LEU:HA     | 1.64                     | 0.46              |
| 5:E:18:ARG:O       | 5:E:22:ILE:HG13    | 2.16                     | 0.46              |
| 5:E:77:GLU:C       | 5:E:79:PHE:N       | 2.74                     | 0.46              |
| 5:E:79:PHE:C       | 5:E:81:GLU:N       | 2.72                     | 0.46              |
| 1:a:5218:LEU:O     | 1:a:5219:VAL:C     | 2.59                     | 0.46              |
| 1:a:5288:LEU:HD13  | 3:c:5432:VAL:HG23  | 1.98                     | 0.46              |
| 22:a:6007:CLA:C9   | 8:i:5016:VAL:HG11  | 2.45                     | 0.46              |
| 2:b:5068:ARG:NH1   | 2:b:5167:TRP:O     | 2.49                     | 0.46              |
| 2:b:5237:VAL:C     | 22:b:6020:CLA:CMD  | 2.89                     | 0.46              |
| 2:b:5248:ALA:HA    | 22:b:6011:CLA:C5   | 2.45                     | 0.46              |
| 2:b:5271:THR:H     | 2:b:5274:GLN:NE2   | 2.13                     | 0.46              |
| 2:b:5290:ALA:O     | 2:b:5294:SER:HB2   | 2.16                     | 0.46              |
| 22:b:6011:CLA:O1D  | 22:b:6013:CLA:C2   | 2.63                     | 0.46              |
| 22:b:6015:CLA:CBB  | 22:b:6015:CLA:HHC  | 2.46                     | 0.46              |
| 28:b:6060:MGE:H102 | 28:b:6060:MGE:H7A1 | 1.31                     | 0.46              |
| 3:c:5063:TRP:NE1   | 22:c:6028:CLA:HMC1 | 2.31                     | 0.46              |
| 3:c:5142:GLU:OE2   | 3:c:5143:TYR:HB2   | 2.16                     | 0.46              |
| 3:c:5178:LYS:HA    | 3:c:5182:PHE:HB2   | 1.98                     | 0.46              |
| 3:c:5376:ASP:OD1   | 3:c:5378:ASN:HB2   | 2.15                     | 0.46              |
| 4:d:5274:VAL:HB    | 4:d:5275:PRO:CD    | 2.38                     | 0.46              |
| 4:d:5297:ASP:O     | 4:d:5298:PHE:HB2   | 2.15                     | 0.46              |
| 4:d:5314:PHE:O     | 4:d:5318:ASN:N     | 2.44                     | 0.46              |
| 4:d:5329:MET:O     | 4:d:5330:ALA:C     | 2.59                     | 0.46              |
| 8:i:5016:VAL:O     | 8:i:5019:PHE:HB3   | 2.16                     | 0.46              |
| 10:k:5028:ILE:HA   | 10:k:5031:LEU:CG   | 2.45                     | 0.46              |
| 13:o:5071:LEU:HB3  | 13:o:5241:PHE:CE2  | 2.50                     | 0.46              |
| 13:o:5184:ASP:OD2  | 13:o:5188:ARG:HB2  | 2.15                     | 0.46              |
| 16:v:5063:CYS:SG   | 16:v:5129:LYS:NZ   | 2.72                     | 0.46              |
| 16:v:5105:PRO:HD3  | 16:v:5120:SER:CB   | 2.46                     | 0.46              |
| 1:A:45:THR:CG2     | 1:A:46:ILE:H       | 2.27                     | 0.46              |
| 1:A:107:TYR:C      | 1:A:109:GLY:N      | 2.74                     | 0.46              |
| 1:A:288:LEU:HD13   | 3:C:432:VAL:HG23   | 1.98                     | 0.46              |
| 1:A:316:THR:C      | 1:A:318:ALA:N      | 2.72                     | 0.46              |
| 2:B:171:PRO:CB     | 2:B:279:TYR:OH     | 2.64                     | 0.46              |
| 3:C:176:VAL:O      | 3:C:180:MET:N      | 2.45                     | 0.46              |
| 3:C:237:HIS:O      | 3:C:238:ILE:C      | 2.58                     | 0.46              |
| 3:C:386:PRO:C      | 3:C:388:GLN:N      | 2.73                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:C:1056:DGD:HAG1 | 29:C:1057:DGD:HA92 | 1.98                     | 0.46              |
| 4:D:147:SER:OG     | 4:D:280:TRP:NE1    | 2.44                     | 0.46              |
| 6:F:24:HIS:O       | 6:F:25:THR:C       | 2.59                     | 0.46              |
| 6:F:37:ILE:HG22    | 9:J:28:PHE:HE1     | 1.81                     | 0.46              |
| 12:M:32:GLN:HA     | 12:M:32:GLN:NE2    | 2.27                     | 0.46              |
| 13:O:116:ASP:OD2   | 13:O:116:ASP:O     | 2.34                     | 0.46              |
| 13:O:216:PHE:HD2   | 13:O:217:SER:N     | 2.14                     | 0.46              |
| 15:U:28:ASN:ND2    | 15:U:55:TYR:N      | 2.62                     | 0.46              |
| 20:Z:32:ASP:HB3    | 20:Z:35:ARG:CG     | 2.46                     | 0.46              |
| 1:a:5209:ALA:HB2   | 4:d:5204:VAL:O     | 2.15                     | 0.46              |
| 2:b:5062:VAL:HG13  | 22:b:6013:CLA:HED2 | 1.95                     | 0.46              |
| 2:b:5149:LEU:HD22  | 22:b:6012:CLA:H203 | 1.97                     | 0.46              |
| 2:b:5171:PRO:CB    | 2:b:5279:TYR:OH    | 2.64                     | 0.46              |
| 2:b:5326:ARG:HH11  | 4:d:5297:ASP:CA    | 2.11                     | 0.46              |
| 2:b:5346:PHE:CD1   | 2:b:5399:VAL:HG22  | 2.51                     | 0.46              |
| 2:b:5360:PRO:HG2   | 2:b:5363:PHE:CD2   | 2.50                     | 0.46              |
| 2:b:5364:GLU:HG3   | 4:d:5296:TYR:CD2   | 2.51                     | 0.46              |
| 22:b:6018:CLA:H202 | 22:b:6018:CLA:H161 | 1.68                     | 0.46              |
| 22:b:6020:CLA:H41  | 22:b:6020:CLA:C8   | 2.45                     | 0.46              |
| 3:c:5029:GLU:OE1   | 3:c:5030:SER:N     | 2.49                     | 0.46              |
| 3:c:5059:LEU:HD11  | 10:k:5032:PHE:CE1  | 2.51                     | 0.46              |
| 3:c:5225:VAL:HG23  | 3:c:5226:SER:H     | 1.80                     | 0.46              |
| 3:c:5305:THR:HG22  | 3:c:5308:GLU:CB    | 2.41                     | 0.46              |
| 3:c:5369:LEU:HD11  | 3:c:5384:ILE:CG1   | 2.46                     | 0.46              |
| 22:c:6035:CLA:H111 | 25:k:6052:BCR:H24C | 1.98                     | 0.46              |
| 29:c:6056:DGD:O1A  | 29:c:6056:DGD:HA52 | 2.16                     | 0.46              |
| 4:d:5113:PHE:O     | 4:d:5114:ILE:C     | 2.57                     | 0.46              |
| 4:d:5144:ILE:O     | 4:d:5145:ALA:C     | 2.59                     | 0.46              |
| 4:d:5147:SER:OG    | 4:d:5280:TRP:NE1   | 2.44                     | 0.46              |
| 4:d:5209:LEU:O     | 4:d:5210:LEU:C     | 2.59                     | 0.46              |
| 4:d:5250:ASN:HD21  | 14:t:5027:PRO:HG3  | 1.81                     | 0.46              |
| 4:d:5269:PHE:CD1   | 4:d:5269:PHE:C     | 2.92                     | 0.46              |
| 9:j:5023:VAL:HG13  | 9:j:5024:ILE:N     | 2.30                     | 0.46              |
| 15:u:5073:GLN:O    | 15:u:5074:ILE:C    | 2.59                     | 0.46              |
| 16:v:5083:GLU:O    | 16:v:5087:LEU:HG   | 2.15                     | 0.46              |
| 20:z:5032:ASP:HB3  | 20:z:5035:ARG:CG   | 2.46                     | 0.46              |
| 1:A:61:ASP:HB2     | 1:A:63:ILE:HD13    | 1.96                     | 0.46              |
| 1:A:269:ARG:HD2    | 4:D:231:THR:O      | 2.16                     | 0.46              |
| 22:B:1009:CLA:OBD  | 22:B:1010:CLA:CBB  | 2.55                     | 0.46              |
| 3:C:36:TRP:O       | 22:C:1032:CLA:H42  | 2.16                     | 0.46              |
| 3:C:42:LEU:HD22    | 22:C:1035:CLA:HMA3 | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:49:LEU:CD2     | 22:C:1035:CLA:CMA  | 2.90                     | 0.46              |
| 3:C:93:ALA:HB1     | 3:C:99:VAL:HG21    | 1.96                     | 0.46              |
| 3:C:142:GLU:OE2    | 3:C:143:TYR:HB2    | 2.16                     | 0.46              |
| 3:C:271:TYR:O      | 3:C:275:SER:HB2    | 2.16                     | 0.46              |
| 3:C:374:GLY:HA2    | 13:O:33:TYR:CE1    | 2.51                     | 0.46              |
| 22:C:1033:CLA:HAA2 | 22:C:1033:CLA:HBD  | 1.97                     | 0.46              |
| 22:C:1036:CLA:CED  | 22:C:1037:CLA:HBB2 | 2.46                     | 0.46              |
| 4:D:14:TRP:O       | 4:D:17:ILE:HG13    | 2.16                     | 0.46              |
| 4:D:29:PHE:CD2     | 4:D:29:PHE:C       | 2.93                     | 0.46              |
| 4:D:183:LEU:H      | 4:D:183:LEU:CD2    | 2.18                     | 0.46              |
| 6:F:19:ARG:HH21    | 6:F:20:TRP:CD1     | 2.34                     | 0.46              |
| 7:H:30:LEU:O       | 7:H:34:PHE:HD2     | 1.98                     | 0.46              |
| 10:K:21:LEU:C      | 10:K:23:ASP:N      | 2.70                     | 0.46              |
| 1:a:5081:ALA:HB2   | 1:a:5175:GLY:HA3   | 1.98                     | 0.46              |
| 1:a:5119:PHE:C     | 1:a:5121:LEU:N     | 2.71                     | 0.46              |
| 2:b:5122:LEU:HD23  | 7:h:5008:GLY:C     | 2.41                     | 0.46              |
| 2:b:5171:PRO:HB3   | 2:b:5279:TYR:OH    | 2.15                     | 0.46              |
| 2:b:5401:PHE:CE1   | 2:b:5406:LEU:HD23  | 2.51                     | 0.46              |
| 2:b:5474:LEU:C     | 2:b:5475:PHE:HD2   | 2.23                     | 0.46              |
| 22:b:6012:CLA:C2D  | 22:b:6020:CLA:H203 | 2.39                     | 0.46              |
| 22:b:6023:CLA:C1D  | 22:b:6024:CLA:HMC3 | 2.45                     | 0.46              |
| 3:c:5185:LEU:CG    | 3:c:5199:ILE:HD11  | 2.38                     | 0.46              |
| 3:c:5223:TRP:CD1   | 3:c:5224:ILE:HD13  | 2.51                     | 0.46              |
| 3:c:5259:TRP:CE3   | 3:c:5260:ALA:N     | 2.84                     | 0.46              |
| 3:c:5266:TRP:HB3   | 3:c:5271:TYR:HH    | 1.79                     | 0.46              |
| 3:c:5284:PHE:CB    | 29:c:6055:DGD:HB71 | 2.44                     | 0.46              |
| 3:c:5321:ASP:C     | 3:c:5324:LEU:H     | 2.23                     | 0.46              |
| 22:c:6028:CLA:O1D  | 29:c:6056:DGD:HE62 | 2.15                     | 0.46              |
| 29:c:6056:DGD:HD62 | 29:c:6056:DGD:C4E  | 2.43                     | 0.46              |
| 29:c:6056:DGD:HAG1 | 29:c:6057:DGD:HA92 | 1.98                     | 0.46              |
| 4:d:5053:THR:CG2   | 4:d:5067:TYR:CD2   | 2.99                     | 0.46              |
| 4:d:5057:SER:HB3   | 4:d:5065:SER:OG    | 2.15                     | 0.46              |
| 4:d:5170:ALA:O     | 4:d:5171:PRO:C     | 2.57                     | 0.46              |
| 4:d:5307:GLU:O     | 4:d:5308:ASP:C     | 2.58                     | 0.46              |
| 4:d:5319:LEU:O     | 4:d:5319:LEU:HD23  | 2.15                     | 0.46              |
| 9:j:5031:GLY:O     | 9:j:5035:GLY:CA    | 2.58                     | 0.46              |
| 10:k:5035:LEU:O    | 10:k:5036:ALA:C    | 2.58                     | 0.46              |
| 11:l:5026:VAL:O    | 11:l:5027:LEU:C    | 2.58                     | 0.46              |
| 13:o:5048:LEU:O    | 13:o:5229:LYS:HD3  | 2.15                     | 0.46              |
| 13:o:5116:ASP:OD2  | 13:o:5116:ASP:O    | 2.34                     | 0.46              |
| 13:o:5151:LEU:HG   | 13:o:5152:VAL:N    | 2.31                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:u:5027:LEU:HD21 | 15:u:5082:PHE:CD1  | 2.46                     | 0.46              |
| 15:u:5032:ILE:HG13 | 15:u:5050:VAL:HG21 | 1.98                     | 0.46              |
| 1:A:31:GLY:HA3     | 1:A:132:GLU:OE2    | 2.16                     | 0.46              |
| 1:A:279:ARG:CZ     | 23:A:1038:PHO:CMC  | 2.90                     | 0.46              |
| 1:A:305:SER:HA     | 9:J:39:SER:HB3     | 1.97                     | 0.46              |
| 2:B:52:LEU:C       | 2:B:54:PRO:HD3     | 2.40                     | 0.46              |
| 2:B:68:ARG:NH1     | 2:B:167:TRP:O      | 2.49                     | 0.46              |
| 2:B:122:LEU:HD23   | 7:H:8:GLY:C        | 2.41                     | 0.46              |
| 2:B:364:GLU:HG3    | 4:D:296:TYR:CD2    | 2.51                     | 0.46              |
| 22:B:1011:CLA:O1D  | 22:B:1013:CLA:C2   | 2.64                     | 0.46              |
| 22:B:1012:CLA:C2D  | 22:B:1020:CLA:H203 | 2.39                     | 0.46              |
| 22:B:1015:CLA:H3A  | 22:B:1015:CLA:HBA2 | 1.55                     | 0.46              |
| 22:B:1016:CLA:H92  | 22:H:1017:CLA:H111 | 1.98                     | 0.46              |
| 25:B:1047:BCR:H272 | 25:t:1046:BCR:C34  | 2.46                     | 0.46              |
| 3:C:29:GLU:OE1     | 3:C:30:SER:N       | 2.49                     | 0.46              |
| 3:C:362:ARG:NE     | 3:C:367:GLU:OE1    | 2.48                     | 0.46              |
| 22:C:1031:CLA:H121 | 22:C:1031:CLA:H161 | 1.62                     | 0.46              |
| 4:D:302:GLU:HA     | 4:D:305:ALA:CB     | 2.46                     | 0.46              |
| 4:D:348:ARG:HH21   | 4:D:352:LEU:C      | 2.22                     | 0.46              |
| 23:D:1039:PHO:HHB  | 22:D:1004:CLA:H121 | 1.98                     | 0.46              |
| 5:E:37:PHE:CE1     | 5:E:43:ALA:HA      | 2.50                     | 0.46              |
| 8:I:4:LEU:O        | 8:I:7:THR:OG1      | 2.26                     | 0.46              |
| 8:I:16:VAL:O       | 8:I:19:PHE:HB3     | 2.16                     | 0.46              |
| 9:J:10:LEU:H       | 9:J:10:LEU:CD1     | 2.10                     | 0.46              |
| 15:U:35:PHE:HE1    | 15:U:49:ILE:HB     | 1.80                     | 0.46              |
| 17:X:44:ASP:OD1    | 17:X:44:ASP:O      | 2.34                     | 0.46              |
| 1:a:5047:CYS:SG    | 1:a:5115:ILE:CD1   | 3.04                     | 0.46              |
| 1:a:5193:LEU:HD22  | 4:d:5179:PHE:CE2   | 2.50                     | 0.46              |
| 2:b:5027:THR:CG2   | 2:b:5107:LEU:HD13  | 2.45                     | 0.46              |
| 2:b:5046:ASP:H     | 2:b:5058:GLN:HE22  | 1.63                     | 0.46              |
| 2:b:5172:TYR:CG    | 2:b:5173:GLY:N     | 2.84                     | 0.46              |
| 2:b:5377:VAL:HG11  | 4:d:5342:PRO:HG2   | 1.97                     | 0.46              |
| 22:b:6012:CLA:CHD  | 22:b:6020:CLA:C20  | 2.94                     | 0.46              |
| 22:b:6015:CLA:H3A  | 22:b:6015:CLA:HBA2 | 1.55                     | 0.46              |
| 22:b:6023:CLA:H151 | 22:b:6024:CLA:NA   | 2.31                     | 0.46              |
| 3:c:5165:LEU:O     | 3:c:5244:CYS:SG    | 2.73                     | 0.46              |
| 3:c:5398:HIS:H     | 3:c:5398:HIS:HD1   | 1.62                     | 0.46              |
| 4:d:5089:LEU:CD1   | 7:h:5050:ASN:OD1   | 2.62                     | 0.46              |
| 7:h:5013:PRO:CG    | 7:h:5014:LEU:HD12  | 2.29                     | 0.46              |
| 7:h:5030:LEU:O     | 7:h:5034:PHE:HD2   | 1.99                     | 0.46              |
| 9:j:5030:TYR:O     | 9:j:5032:ALA:N     | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5041:LEU:C    | 13:o:5043:ASN:H    | 2.24                     | 0.46              |
| 13:o:5104:LEU:HD12 | 13:o:5104:LEU:C    | 2.40                     | 0.46              |
| 13:o:5216:PHE:HD2  | 13:o:5217:SER:N    | 2.14                     | 0.46              |
| 15:u:5051:LYS:O    | 15:u:5052:ASN:HB2  | 2.15                     | 0.46              |
| 16:v:5034:LEU:CD2  | 16:v:5047:LEU:HB3  | 2.30                     | 0.46              |
| 1:A:39:PRO:CD      | 22:A:1007:CLA:HBB2 | 2.45                     | 0.46              |
| 1:A:204:GLY:O      | 1:A:207:GLY:N      | 2.48                     | 0.46              |
| 1:A:210:LEU:HA     | 23:D:1039:PHO:CBC  | 2.46                     | 0.46              |
| 1:A:340:PRO:HD3    | 15:U:103:TYR:HE2   | 1.77                     | 0.46              |
| 2:B:49:ASP:CA      | 13:o:5083:LYS:HE3  | 2.45                     | 0.46              |
| 2:B:360:PRO:HG2    | 2:B:363:PHE:CE2    | 2.52                     | 0.46              |
| 22:B:1015:CLA:H18  | 28:B:1060:MGE:CCA  | 2.46                     | 0.46              |
| 22:B:1018:CLA:C8   | 22:B:1023:CLA:CBA  | 2.94                     | 0.46              |
| 3:C:272:LEU:HD12   | 3:C:276:LEU:HB2    | 1.98                     | 0.46              |
| 3:C:398:HIS:HD1    | 3:C:398:HIS:H      | 1.62                     | 0.46              |
| 29:C:1056:DGD:HD62 | 29:C:1056:DGD:C4E  | 2.43                     | 0.46              |
| 4:D:191:TRP:O      | 4:D:194:ASN:N      | 2.49                     | 0.46              |
| 4:D:218:VAL:HG22   | 4:D:244:TYR:CD1    | 2.51                     | 0.46              |
| 4:D:230:SER:C      | 4:D:232:PHE:N      | 2.74                     | 0.46              |
| 4:D:250:ASN:HD21   | 14:T:27:PRO:HG3    | 1.81                     | 0.46              |
| 4:D:274:VAL:CB     | 4:D:275:PRO:CD     | 2.94                     | 0.46              |
| 11:L:25:LEU:HD12   | 14:T:16:LEU:HD22   | 1.97                     | 0.46              |
| 12:M:29:THR:C      | 12:M:31:SER:H      | 2.24                     | 0.46              |
| 1:a:5039:PRO:O     | 1:a:5040:THR:C     | 2.59                     | 0.46              |
| 1:a:5045:THR:CG2   | 1:a:5046:ILE:H     | 2.27                     | 0.46              |
| 1:a:5107:TYR:C     | 1:a:5109:GLY:N     | 2.74                     | 0.46              |
| 1:a:5192:ILE:CG2   | 1:a:5193:LEU:N     | 2.79                     | 0.46              |
| 1:a:5271:LEU:O     | 1:a:5272:HIS:C     | 2.59                     | 0.46              |
| 2:b:5135:LEU:HB2   | 22:b:6018:CLA:HBC1 | 1.98                     | 0.46              |
| 3:c:5033:PHE:CD2   | 4:d:5229:ALA:HB1   | 2.51                     | 0.46              |
| 3:c:5160:ILE:O     | 3:c:5161:LEU:C     | 2.57                     | 0.46              |
| 3:c:5172:ALA:H     | 22:c:6025:CLA:HBC2 | 1.76                     | 0.46              |
| 3:c:5257:PHE:HD1   | 3:c:5257:PHE:N     | 2.09                     | 0.46              |
| 3:c:5274:TYR:O     | 3:c:5275:SER:C     | 2.59                     | 0.46              |
| 22:c:6028:CLA:H91  | 29:c:6056:DGD:HB91 | 1.98                     | 0.46              |
| 22:c:6035:CLA:CMB  | 25:k:6052:BCR:H272 | 2.45                     | 0.46              |
| 22:c:6037:CLA:H3A  | 22:c:6037:CLA:HBA2 | 1.44                     | 0.46              |
| 4:d:5067:TYR:O     | 4:d:5070:GLY:N     | 2.47                     | 0.46              |
| 4:d:5087:HIS:HA    | 4:d:5167:TRP:NE1   | 2.31                     | 0.46              |
| 4:d:5302:GLU:HA    | 4:d:5305:ALA:CB    | 2.46                     | 0.46              |
| 10:k:5032:PHE:CZ   | 25:k:6052:BCR:C36  | 2.82                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:l:5013:ASN:O    | 11:l:5015:THR:N    | 2.48                     | 0.46              |
| 11:l:5025:LEU:HD12 | 14:t:5016:LEU:HD22 | 1.97                     | 0.46              |
| 13:o:5052:ALA:O    | 13:o:5053:ARG:HB3  | 2.15                     | 0.46              |
| 13:o:5059:ASP:O    | 13:o:5060:SER:HB2  | 2.16                     | 0.46              |
| 13:o:5163:THR:C    | 13:o:5165:SER:N    | 2.72                     | 0.46              |
| 15:u:5028:ASN:ND2  | 15:u:5055:TYR:N    | 2.62                     | 0.46              |
| 16:v:5035:THR:CA   | 16:v:5046:THR:HA   | 2.43                     | 0.46              |
| 1:A:47:CYS:SG      | 1:A:115:ILE:CD1    | 3.04                     | 0.45              |
| 1:A:143:ILE:HB     | 4:D:220:ASN:HD22   | 1.79                     | 0.45              |
| 1:A:157:VAL:O      | 1:A:158:PHE:CD2    | 2.69                     | 0.45              |
| 1:A:210:LEU:HD22   | 1:A:211:PHE:CD2    | 2.51                     | 0.45              |
| 2:B:122:LEU:HD23   | 7:H:8:GLY:CA       | 2.46                     | 0.45              |
| 2:B:140:GLY:O      | 2:B:143:LEU:HB3    | 2.16                     | 0.45              |
| 2:B:231:MET:HG2    | 22:B:1018:CLA:HAC2 | 1.98                     | 0.45              |
| 2:B:456:ALA:HB1    | 29:B:1058:DGD:CHB  | 2.28                     | 0.45              |
| 22:B:1011:CLA:C2D  | 22:B:1013:CLA:H12  | 2.45                     | 0.45              |
| 22:B:1016:CLA:H93  | 22:B:1016:CLA:H61  | 1.64                     | 0.45              |
| 3:C:60:ILE:HG13    | 22:C:1027:CLA:CMD  | 2.46                     | 0.45              |
| 3:C:128:GLY:HA3    | 22:C:1037:CLA:C3C  | 2.46                     | 0.45              |
| 3:C:131:TYR:CG     | 3:C:132:HIS:N      | 2.83                     | 0.45              |
| 3:C:206:PRO:O      | 3:C:210:PHE:HB2    | 2.16                     | 0.45              |
| 3:C:348:GLU:HG2    | 3:C:349:ILE:CG1    | 2.36                     | 0.45              |
| 4:D:87:HIS:HA      | 4:D:167:TRP:NE1    | 2.31                     | 0.45              |
| 4:D:126:MET:O      | 4:D:129:GLN:HB2    | 2.16                     | 0.45              |
| 4:D:144:ILE:O      | 4:D:145:ALA:C      | 2.59                     | 0.45              |
| 7:H:12:ARG:N       | 7:H:13:PRO:CD      | 2.79                     | 0.45              |
| 7:H:17:GLU:CB      | 7:H:20:LYS:HD3     | 2.45                     | 0.45              |
| 9:J:23:VAL:HG13    | 9:J:24:ILE:N       | 2.30                     | 0.45              |
| 9:J:38:SER:O       | 9:J:39:SER:OG      | 2.31                     | 0.45              |
| 1:a:5013:LEU:H     | 1:a:5013:LEU:CD1   | 2.27                     | 0.45              |
| 1:a:5031:GLY:HA3   | 1:a:5132:GLU:OE2   | 2.16                     | 0.45              |
| 1:a:5204:GLY:O     | 1:a:5205:VAL:C     | 2.58                     | 0.45              |
| 1:a:5323:ARG:HD2   | 1:a:5323:ARG:HA    | 1.72                     | 0.45              |
| 2:b:5151:PHE:HB2   | 2:b:5206:GLY:HA3   | 1.98                     | 0.45              |
| 2:b:5247:PHE:CE1   | 22:b:6010:CLA:H93  | 2.51                     | 0.45              |
| 2:b:5321:LYS:O     | 2:b:5322:GLY:O     | 2.34                     | 0.45              |
| 2:b:5350:GLU:N     | 2:b:5350:GLU:OE2   | 2.49                     | 0.45              |
| 2:b:5360:PRO:HG2   | 2:b:5363:PHE:CE2   | 2.52                     | 0.45              |
| 22:b:6011:CLA:H2   | 22:b:6013:CLA:H91  | 1.93                     | 0.45              |
| 22:b:6018:CLA:H2   | 22:b:6018:CLA:H111 | 1.97                     | 0.45              |
| 22:b:6022:CLA:CBC  | 22:b:6022:CLA:CHD  | 2.79                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6023:CLA:H91  | 22:b:6024:CLA:H152 | 1.88                     | 0.45              |
| 3:c:5060:ILE:HG13  | 22:c:6027:CLA:CMD  | 2.46                     | 0.45              |
| 3:c:5371:GLY:N     | 3:c:5374:GLY:O     | 2.49                     | 0.45              |
| 22:c:6027:CLA:HBB1 | 22:c:6027:CLA:HHC  | 1.98                     | 0.45              |
| 4:d:5057:SER:OG    | 4:d:5065:SER:CB    | 2.64                     | 0.45              |
| 4:d:5180:ARG:HD2   | 4:d:5180:ARG:C     | 2.41                     | 0.45              |
| 4:d:5199:MET:HE3   | 24:d:6042:PQ9:H352 | 1.96                     | 0.45              |
| 5:e:5018:ARG:O     | 5:e:5022:ILE:HG13  | 2.16                     | 0.45              |
| 5:e:5026:THR:HG22  | 19:n:5014:UNK:O    | 2.15                     | 0.45              |
| 10:k:5033:PHE:HE1  | 10:k:5037:PHE:CD2  | 2.34                     | 0.45              |
| 15:u:5028:ASN:ND2  | 15:u:5054:PRO:HB2  | 2.24                     | 0.45              |
| 1:A:187:GLN:CG     | 1:A:325:ASN:HD21   | 2.17                     | 0.45              |
| 1:A:205:VAL:HA     | 1:A:279:ARG:HH21   | 1.81                     | 0.45              |
| 1:A:288:LEU:HD22   | 3:C:432:VAL:HA     | 1.98                     | 0.45              |
| 1:A:323:ARG:C      | 1:A:325:ASN:N      | 2.73                     | 0.45              |
| 2:B:7:ARG:NH1      | 2:B:7:ARG:CG       | 2.58                     | 0.45              |
| 2:B:27:THR:CG2     | 2:B:107:LEU:HD13   | 2.45                     | 0.45              |
| 2:B:135:LEU:HB2    | 22:B:1018:CLA:HBC1 | 1.98                     | 0.45              |
| 2:B:149:LEU:HD22   | 22:B:1012:CLA:H203 | 1.97                     | 0.45              |
| 2:B:401:PHE:CE1    | 2:B:406:LEU:HD23   | 2.51                     | 0.45              |
| 22:B:1022:CLA:CGD  | 22:B:1022:CLA:CAA  | 2.65                     | 0.45              |
| 22:B:1023:CLA:C1D  | 22:B:1024:CLA:HMC3 | 2.45                     | 0.45              |
| 3:C:284:PHE:CE1    | 3:C:431:PHE:CD2    | 3.03                     | 0.45              |
| 3:C:334:PRO:HG2    | 4:D:350:ASN:ND2    | 2.31                     | 0.45              |
| 3:C:456:GLU:H      | 3:C:456:GLU:HG3    | 1.42                     | 0.45              |
| 22:C:1029:CLA:H92  | 22:C:1029:CLA:H62  | 1.80                     | 0.45              |
| 22:C:1036:CLA:H3A  | 22:C:1036:CLA:HBA1 | 1.59                     | 0.45              |
| 4:D:189:HIS:ND1    | 4:D:294:ARG:HD3    | 2.31                     | 0.45              |
| 4:D:214:HIS:C      | 4:D:217:THR:HG22   | 2.41                     | 0.45              |
| 4:D:267:LEU:CD2    | 4:D:268:HIS:ND1    | 2.62                     | 0.45              |
| 5:E:24:SER:O       | 5:E:28:PRO:HD2     | 2.17                     | 0.45              |
| 25:H:1049:BCR:H24C | 25:H:1049:BCR:H371 | 1.63                     | 0.45              |
| 9:J:30:TYR:O       | 9:J:32:ALA:N       | 2.49                     | 0.45              |
| 13:O:48:LEU:O      | 13:O:229:LYS:HD3   | 2.15                     | 0.45              |
| 13:O:71:LEU:HB3    | 13:O:241:PHE:CE2   | 2.51                     | 0.45              |
| 13:O:210:ARG:NE    | 13:O:252:GLY:O     | 2.49                     | 0.45              |
| 16:V:103:LYS:HE3   | 16:V:138:LEU:HD12  | 1.97                     | 0.45              |
| 17:X:39:ALA:O      | 17:X:43:ILE:HD13   | 2.15                     | 0.45              |
| 18:Y:39:LEU:HD21   | 20:Z:25:VAL:HA     | 1.98                     | 0.45              |
| 1:a:5107:TYR:CD2   | 13:o:5097:VAL:CG1  | 2.99                     | 0.45              |
| 1:a:5290:ILE:HA    | 1:a:5290:ILE:HD12  | 1.65                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:a:6007:CLA:H193 | 22:a:6007:CLA:H162 | 1.73                     | 0.45              |
| 2:b:5033:TRP:O     | 2:b:5036:SER:HB2   | 2.15                     | 0.45              |
| 2:b:5047:PRO:HB3   | 2:b:5078:TRP:CE3   | 2.51                     | 0.45              |
| 2:b:5122:LEU:HD23  | 7:h:5008:GLY:CA    | 2.46                     | 0.45              |
| 2:b:5153:PHE:O     | 2:b:5154:GLY:C     | 2.59                     | 0.45              |
| 22:b:6010:CLA:CMD  | 22:b:6011:CLA:H92  | 2.46                     | 0.45              |
| 22:b:6013:CLA:C17  | 22:b:6013:CLA:C14  | 2.93                     | 0.45              |
| 22:c:6035:CLA:H143 | 22:c:6035:CLA:H112 | 1.79                     | 0.45              |
| 4:d:5129:GLN:O     | 4:d:5133:ALA:HB2   | 2.16                     | 0.45              |
| 4:d:5170:ALA:C     | 4:d:5171:PRO:O     | 2.59                     | 0.45              |
| 4:d:5308:ASP:O     | 4:d:5310:GLU:N     | 2.50                     | 0.45              |
| 5:e:5008:ARG:HB2   | 6:f:5013:TYR:HB3   | 1.98                     | 0.45              |
| 5:e:5063:ILE:HA    | 5:e:5064:PRO:HD3   | 1.76                     | 0.45              |
| 7:h:5044:ILE:HD13  | 7:h:5044:ILE:HA    | 1.77                     | 0.45              |
| 10:k:5021:LEU:C    | 10:k:5023:ASP:N    | 2.70                     | 0.45              |
| 22:k:6034:CLA:H43  | 22:k:6034:CLA:CBA  | 2.44                     | 0.45              |
| 18:y:5043:ARG:HH21 | 18:y:5044:GLY:N    | 2.14                     | 0.45              |
| 1:A:129:ARG:CZ     | 4:D:256:ILE:CD1    | 2.91                     | 0.45              |
| 1:A:252:HIS:CD2    | 1:A:264:SER:HB3    | 2.51                     | 0.45              |
| 1:A:259:ILE:CD1    | 24:A:1043:PQ9:H242 | 2.37                     | 0.45              |
| 1:A:304:HIS:CD2    | 3:C:414:ILE:HD13   | 2.52                     | 0.45              |
| 2:B:47:PRO:HB3     | 2:B:78:TRP:CE3     | 2.51                     | 0.45              |
| 2:B:65:PHE:HZ      | 22:B:1012:CLA:HMA3 | 1.72                     | 0.45              |
| 2:B:247:PHE:CE1    | 22:B:1010:CLA:H93  | 2.51                     | 0.45              |
| 2:B:317:ASN:O      | 2:B:319:PRO:HD3    | 2.16                     | 0.45              |
| 2:B:346:PHE:CD1    | 2:B:399:VAL:HG22   | 2.51                     | 0.45              |
| 22:B:1023:CLA:CHD  | 22:B:1024:CLA:HBC2 | 2.46                     | 0.45              |
| 3:C:62:PHE:HE2     | 10:K:29:PRO:HD3    | 1.81                     | 0.45              |
| 3:C:404:LEU:C      | 3:C:406:SER:N      | 2.73                     | 0.45              |
| 3:C:431:PHE:C      | 3:C:431:PHE:HD2    | 2.23                     | 0.45              |
| 4:D:103:ARG:HG3    | 5:E:73:LYS:HD3     | 1.97                     | 0.45              |
| 4:D:221:THR:O      | 4:D:244:TYR:CA     | 2.64                     | 0.45              |
| 4:D:315:TYR:O      | 4:D:319:LEU:HB2    | 2.16                     | 0.45              |
| 6:F:29:PRO:O       | 6:F:30:THR:C       | 2.58                     | 0.45              |
| 13:O:79:LYS:CE     | 13:O:89:ALA:HB3    | 2.47                     | 0.45              |
| 13:O:227:VAL:HG11  | 13:O:230:VAL:CG2   | 2.45                     | 0.45              |
| 15:U:51:LYS:HG3    | 15:U:52:ASN:N      | 2.23                     | 0.45              |
| 15:U:75:LEU:O      | 15:U:76:ARG:C      | 2.59                     | 0.45              |
| 16:V:63:CYS:SG     | 16:V:129:LYS:NZ    | 2.72                     | 0.45              |
| 1:a:5032:TRP:HA    | 1:a:5032:TRP:CE3   | 2.50                     | 0.45              |
| 1:a:5038:ILE:HG22  | 1:a:5039:PRO:CD    | 2.46                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5157:VAL:O     | 1:a:5158:PHE:CD2   | 2.69                     | 0.45              |
| 1:a:5304:HIS:CD2   | 3:c:5414:ILE:HD13  | 2.52                     | 0.45              |
| 2:b:5106:LEU:O     | 2:b:5109:LEU:N     | 2.48                     | 0.45              |
| 22:b:6016:CLA:C15  | 22:d:6008:CLA:HMA1 | 2.37                     | 0.45              |
| 3:c:5100:GLY:O     | 3:c:5101:PRO:C     | 2.58                     | 0.45              |
| 3:c:5271:TYR:O     | 3:c:5275:SER:HB2   | 2.16                     | 0.45              |
| 3:c:5272:LEU:HD12  | 3:c:5276:LEU:HB2   | 1.98                     | 0.45              |
| 3:c:5348:GLU:OE2   | 3:c:5349:ILE:CG1   | 2.63                     | 0.45              |
| 3:c:5456:GLU:H     | 3:c:5456:GLU:HG3   | 1.42                     | 0.45              |
| 22:c:6036:CLA:CED  | 22:c:6037:CLA:HBB2 | 2.46                     | 0.45              |
| 4:d:5261:PHE:N     | 24:d:6042:PQ9:H91  | 2.14                     | 0.45              |
| 6:f:5024:HIS:C     | 6:f:5026:LEU:N     | 2.73                     | 0.45              |
| 13:o:5136:MET:HE3  | 13:o:5136:MET:HB3  | 1.73                     | 0.45              |
| 1:A:93:PHE:CB      | 3:C:218:PHE:HD2    | 2.28                     | 0.45              |
| 1:A:103:ASP:HA     | 1:A:106:LEU:CD1    | 2.39                     | 0.45              |
| 23:A:1038:PHO:H143 | 23:A:1038:PHO:H161 | 1.62                     | 0.45              |
| 2:B:42:LEU:HD21    | 2:B:93:PHE:HB3     | 1.97                     | 0.45              |
| 2:B:69:LEU:CD2     | 22:B:1013:CLA:O1A  | 2.64                     | 0.45              |
| 2:B:74:SER:HA      | 2:B:92:SER:OG      | 2.16                     | 0.45              |
| 2:B:298:LEU:HD11   | 2:B:302:TRP:NE1    | 2.26                     | 0.45              |
| 2:B:309:LEU:O      | 2:B:309:LEU:HD12   | 2.17                     | 0.45              |
| 2:B:321:LYS:O      | 2:B:322:GLY:O      | 2.34                     | 0.45              |
| 2:B:393:GLU:HG3    | 2:B:414:PRO:HB3    | 1.98                     | 0.45              |
| 22:B:1009:CLA:HED1 | 7:H:41:PHE:CE1     | 2.51                     | 0.45              |
| 3:C:207:ARG:O      | 3:C:211:GLY:HA3    | 2.17                     | 0.45              |
| 3:C:267:SER:O      | 3:C:268:GLY:C      | 2.59                     | 0.45              |
| 3:C:274:TYR:O      | 3:C:275:SER:C      | 2.59                     | 0.45              |
| 3:C:429:SER:O      | 3:C:432:VAL:CG1    | 2.60                     | 0.45              |
| 4:D:129:GLN:O      | 4:D:133:ALA:HB2    | 2.16                     | 0.45              |
| 4:D:170:ALA:O      | 4:D:171:PRO:C      | 2.57                     | 0.45              |
| 4:D:173:PHE:CE1    | 23:D:1039:PHO:H13  | 2.51                     | 0.45              |
| 4:D:209:LEU:O      | 4:D:210:LEU:C      | 2.59                     | 0.45              |
| 4:D:329:MET:O      | 4:D:330:ALA:C      | 2.59                     | 0.45              |
| 6:F:41:GLN:HE22    | 9:J:28:PHE:HA      | 1.74                     | 0.45              |
| 13:O:216:PHE:C     | 13:O:216:PHE:CD2   | 2.94                     | 0.45              |
| 14:T:18:PHE:HD2    | 14:T:19:PHE:CE2    | 2.33                     | 0.45              |
| 15:U:44:THR:O      | 15:U:47:LYS:N      | 2.49                     | 0.45              |
| 1:a:5333:GLU:HB2   | 1:a:5337:HIS:CE1   | 2.51                     | 0.45              |
| 2:b:5024:LEU:HD13  | 22:b:6024:CLA:HBB1 | 1.97                     | 0.45              |
| 2:b:5418:LYS:O     | 2:b:5421:ALA:N     | 2.43                     | 0.45              |
| 22:b:6018:CLA:C8   | 22:b:6023:CLA:CBA  | 2.94                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5039:ASN:CG    | 22:c:6033:CLA:HBB2 | 2.42                     | 0.45              |
| 3:c:5062:PHE:HE2   | 10:k:5029:PRO:HD3  | 1.81                     | 0.45              |
| 3:c:5273:SER:O     | 3:c:5274:TYR:O     | 2.33                     | 0.45              |
| 3:c:5417:VAL:HG11  | 16:v:5068:VAL:HG12 | 1.86                     | 0.45              |
| 22:c:6033:CLA:HMA3 | 22:k:6034:CLA:C3C  | 2.41                     | 0.45              |
| 22:c:6035:CLA:H152 | 20:z:5020:VAL:HG13 | 1.98                     | 0.45              |
| 4:d:5063:LEU:HD23  | 4:d:5064:ALA:N     | 2.32                     | 0.45              |
| 4:d:5079:SER:C     | 4:d:5080:THR:HG22  | 2.42                     | 0.45              |
| 4:d:5214:HIS:CA    | 4:d:5217:THR:HG22  | 2.47                     | 0.45              |
| 4:d:5218:VAL:HG22  | 4:d:5244:TYR:CD1   | 2.52                     | 0.45              |
| 4:d:5319:LEU:O     | 4:d:5322:ASN:HB2   | 2.17                     | 0.45              |
| 22:d:6005:CLA:H91  | 28:d:6062:MGE:H263 | 1.99                     | 0.45              |
| 5:e:5027:ILE:HG13  | 31:f:6040:HEM:CMB  | 2.46                     | 0.45              |
| 5:e:5035:TRP:HA    | 6:f:5039:ALA:HB2   | 1.98                     | 0.45              |
| 8:i:5012:VAL:HG12  | 8:i:5013:THR:N     | 2.31                     | 0.45              |
| 10:k:5028:ILE:HB   | 10:k:5029:PRO:HD3  | 1.97                     | 0.45              |
| 15:u:5029:ASN:O    | 15:u:5030:THR:C    | 2.60                     | 0.45              |
| 15:u:5083:THR:CG2  | 15:u:5084:VAL:H    | 2.25                     | 0.45              |
| 1:A:31:GLY:HA3     | 1:A:132:GLU:CD     | 2.42                     | 0.45              |
| 1:A:215:HIS:HD1    | 24:A:1043:PQ9:H91  | 1.80                     | 0.45              |
| 2:B:24:LEU:HD13    | 22:B:1024:CLA:HBB1 | 1.97                     | 0.45              |
| 2:B:174:LEU:CD2    | 2:B:265:ILE:HB     | 2.46                     | 0.45              |
| 2:B:271:THR:HG22   | 2:B:274:GLN:CD     | 2.41                     | 0.45              |
| 2:B:350:GLU:OE2    | 2:B:350:GLU:N      | 2.49                     | 0.45              |
| 3:C:239:TRP:HE3    | 3:C:243:ILE:HD11   | 1.81                     | 0.45              |
| 3:C:327:ASN:ND2    | 3:C:330:SER:C      | 2.75                     | 0.45              |
| 3:C:349:ILE:CG2    | 3:C:375:LEU:HB2    | 2.44                     | 0.45              |
| 4:D:17:ILE:HD12    | 17:X:41:SER:HG     | 1.82                     | 0.45              |
| 4:D:63:LEU:HD23    | 4:D:64:ALA:N       | 2.32                     | 0.45              |
| 4:D:100:ASP:C      | 4:D:102:THR:H      | 2.25                     | 0.45              |
| 4:D:155:SER:HA     | 4:D:159:ILE:CG1    | 2.47                     | 0.45              |
| 4:D:274:VAL:HB     | 4:D:275:PRO:CD     | 2.38                     | 0.45              |
| 4:D:312:GLU:CG     | 13:O:185:PRO:HB3   | 2.46                     | 0.45              |
| 4:D:314:PHE:O      | 4:D:318:ASN:N      | 2.45                     | 0.45              |
| 4:D:326:ARG:O      | 4:D:328:TRP:N      | 2.49                     | 0.45              |
| 8:I:12:VAL:HG12    | 8:I:13:THR:N       | 2.31                     | 0.45              |
| 10:K:28:ILE:HB     | 10:K:29:PRO:HD3    | 1.97                     | 0.45              |
| 12:M:6:LEU:O       | 12:M:7:GLY:C       | 2.56                     | 0.45              |
| 13:O:252:GLY:O     | 13:O:253:ALA:C     | 2.59                     | 0.45              |
| 16:V:98:LEU:HB3    | 16:V:102:MET:HE2   | 1.97                     | 0.45              |
| 18:Y:42:ARG:HB3    | 18:Y:43:ARG:NE     | 2.28                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:Y:43:ARG:CZ     | 18:Y:43:ARG:H      | 2.30                     | 0.45              |
| 20:Z:20:VAL:O      | 20:Z:21:ILE:C      | 2.58                     | 0.45              |
| 1:a:5278:TRP:CH2   | 29:c:6057:DGD:HAV2 | 2.51                     | 0.45              |
| 2:b:5140:GLY:O     | 2:b:5143:LEU:HB3   | 2.16                     | 0.45              |
| 2:b:5196:GLY:C     | 2:b:5198:VAL:N     | 2.74                     | 0.45              |
| 2:b:5259:GLY:HA3   | 7:h:5062:TRP:CZ2   | 2.52                     | 0.45              |
| 2:b:5393:GLU:HG3   | 2:b:5414:PRO:HB3   | 1.98                     | 0.45              |
| 3:c:5086:LEU:HB3   | 3:c:5090:PRO:HD3   | 1.98                     | 0.45              |
| 22:c:6026:CLA:H122 | 22:c:6026:CLA:C6   | 2.44                     | 0.45              |
| 22:c:6033:CLA:HMA3 | 22:k:6034:CLA:CAC  | 2.42                     | 0.45              |
| 29:c:6057:DGD:CEB  | 29:c:6057:DGD:HBG3 | 2.21                     | 0.45              |
| 4:d:5173:PHE:CE1   | 23:d:6039:PHO:H13  | 2.51                     | 0.45              |
| 4:d:5191:TRP:O     | 4:d:5194:ASN:N     | 2.49                     | 0.45              |
| 4:d:5258:GLY:C     | 4:d:5259:ILE:HD13  | 2.40                     | 0.45              |
| 22:d:6005:CLA:HBC1 | 22:d:6004:CLA:CBB  | 2.34                     | 0.45              |
| 8:i:5027:ASP:C     | 8:i:5029:ALA:N     | 2.73                     | 0.45              |
| 10:k:5028:ILE:HA   | 10:k:5031:LEU:HG   | 1.99                     | 0.45              |
| 13:o:5047:THR:O    | 13:o:5048:LEU:HD23 | 2.16                     | 0.45              |
| 14:t:5009:ILE:O    | 14:t:5010:PHE:C    | 2.59                     | 0.45              |
| 1:A:192:ILE:CG2    | 1:A:193:LEU:N      | 2.79                     | 0.45              |
| 1:A:258:LEU:O      | 1:A:259:ILE:CG1    | 2.64                     | 0.45              |
| 22:A:1003:CLA:H141 | 23:A:1038:PHO:C8   | 2.45                     | 0.45              |
| 24:A:1043:PQ9:H212 | 23:D:1039:PHO:CED  | 2.45                     | 0.45              |
| 2:B:259:GLY:HA3    | 7:H:62:TRP:CZ2     | 2.52                     | 0.45              |
| 28:B:1060:MGE:H7A1 | 28:B:1060:MGE:H102 | 1.31                     | 0.45              |
| 3:C:46:SER:OG      | 3:C:141:GLU:CA     | 2.65                     | 0.45              |
| 3:C:178:LYS:HA     | 3:C:182:PHE:HB2    | 1.98                     | 0.45              |
| 3:C:276:LEU:C      | 3:C:276:LEU:CD2    | 2.88                     | 0.45              |
| 3:C:318:LEU:HA     | 3:C:340:TYR:HD1    | 1.80                     | 0.45              |
| 4:D:49:LEU:HD13    | 25:D:1050:BCR:C14  | 2.47                     | 0.45              |
| 4:D:53:THR:HG23    | 4:D:67:TYR:CD2     | 2.51                     | 0.45              |
| 4:D:185:PHE:CD1    | 4:D:289:LEU:HD13   | 2.52                     | 0.45              |
| 4:D:319:LEU:O      | 4:D:322:ASN:HB2    | 2.17                     | 0.45              |
| 24:D:1042:PQ9:H211 | 24:D:1042:PQ9:H251 | 1.71                     | 0.45              |
| 5:E:35:TRP:HA      | 6:F:39:ALA:HB2     | 1.98                     | 0.45              |
| 5:E:47:PHE:C       | 5:E:49:THR:N       | 2.75                     | 0.45              |
| 13:O:80:GLU:N      | 13:O:90:GLU:O      | 2.48                     | 0.45              |
| 15:U:74:ILE:O      | 15:U:75:LEU:C      | 2.58                     | 0.45              |
| 1:a:5020:TRP:CD1   | 1:a:5026:ASN:HD21  | 2.35                     | 0.45              |
| 1:a:5172:MET:HE2   | 1:a:5179:THR:CA    | 2.46                     | 0.45              |
| 1:a:5269:ARG:HD2   | 4:d:5231:THR:O     | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:a:6043:PQ9:H292 | 24:a:6043:PQ9:H393 | 1.99                     | 0.45              |
| 2:b:5149:LEU:CB    | 22:b:6011:CLA:HBC1 | 2.46                     | 0.45              |
| 2:b:5153:PHE:HD1   | 2:b:5157:HIS:CB    | 2.29                     | 0.45              |
| 22:b:6009:CLA:HED1 | 7:h:5041:PHE:CE1   | 2.51                     | 0.45              |
| 22:b:6015:CLA:H18  | 28:b:6060:MGE:CCA  | 2.46                     | 0.45              |
| 22:b:6022:CLA:C9   | 22:b:6022:CLA:CBC  | 2.62                     | 0.45              |
| 22:b:6023:CLA:CHD  | 22:b:6024:CLA:HBC2 | 2.46                     | 0.45              |
| 3:c:5051:GLY:O     | 3:c:5052:ALA:C     | 2.59                     | 0.45              |
| 3:c:5109:PHE:HB3   | 3:c:5110:PRO:CD    | 2.40                     | 0.45              |
| 3:c:5362:ARG:NE    | 3:c:5367:GLU:OE1   | 2.48                     | 0.45              |
| 3:c:5374:GLY:HA2   | 13:o:5033:TYR:CE1  | 2.51                     | 0.45              |
| 3:c:5448:ALA:C     | 3:c:5450:ALA:N     | 2.75                     | 0.45              |
| 4:d:5308:ASP:C     | 4:d:5310:GLU:N     | 2.72                     | 0.45              |
| 1:A:39:PRO:O       | 1:A:40:THR:C       | 2.59                     | 0.45              |
| 1:A:119:PHE:CZ     | 22:A:1003:CLA:H102 | 2.52                     | 0.45              |
| 1:A:172:MET:HE2    | 1:A:179:THR:CA     | 2.46                     | 0.45              |
| 26:A:1063:LHG:O9   | 26:A:1063:LHG:C6   | 2.52                     | 0.45              |
| 26:A:1063:LHG:H302 | 26:A:1063:LHG:H332 | 1.58                     | 0.45              |
| 2:B:21:ALA:HB2     | 2:B:114:HIS:CB     | 2.47                     | 0.45              |
| 2:B:25:MET:O       | 2:B:27:THR:N       | 2.50                     | 0.45              |
| 2:B:134:ASP:H      | 7:H:15:ASN:ND2     | 2.15                     | 0.45              |
| 22:B:1013:CLA:C17  | 22:B:1013:CLA:C14  | 2.93                     | 0.45              |
| 22:B:1022:CLA:C14  | 22:B:1022:CLA:C7   | 2.70                     | 0.45              |
| 3:C:206:PRO:HG2    | 3:C:207:ARG:HH11   | 1.82                     | 0.45              |
| 4:D:180:ARG:HD2    | 4:D:180:ARG:C      | 2.41                     | 0.45              |
| 4:D:261:PHE:HE2    | 4:D:266:TRP:CD1    | 2.35                     | 0.45              |
| 4:D:331:PRO:HD3    | 4:D:341:PHE:HE2    | 1.82                     | 0.45              |
| 22:D:1008:CLA:HHC  | 22:D:1008:CLA:CBB  | 2.19                     | 0.45              |
| 28:D:1062:MGE:O1A  | 28:D:1062:MGE:C3B  | 2.60                     | 0.45              |
| 25:H:1049:BCR:C40  | 17:X:20:PHE:HZ     | 2.28                     | 0.45              |
| 11:L:15:THR:O      | 11:L:16:SER:C      | 2.60                     | 0.45              |
| 13:O:41:LEU:C      | 13:O:43:ASN:H      | 2.24                     | 0.45              |
| 13:O:83:LYS:CE     | 2:b:5049:ASP:HB2   | 2.46                     | 0.45              |
| 15:U:88:GLU:HB3    | 15:U:91:LEU:HB2    | 1.99                     | 0.45              |
| 17:X:33:THR:HG22   | 17:X:34:PHE:N      | 2.31                     | 0.45              |
| 1:a:5210:LEU:HA    | 23:d:6039:PHO:CBC  | 2.46                     | 0.45              |
| 1:a:5341:LEU:O     | 1:a:5343:LEU:N     | 2.48                     | 0.45              |
| 2:b:5015:ASP:N     | 2:b:5016:PRO:CD    | 2.79                     | 0.45              |
| 2:b:5025:MET:O     | 2:b:5027:THR:N     | 2.50                     | 0.45              |
| 2:b:5181:VAL:HG11  | 2:b:5196:GLY:HA2   | 1.97                     | 0.45              |
| 2:b:5250:PHE:HB3   | 29:b:6058:DGD:HB82 | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5309:LEU:O     | 2:b:5309:LEU:HD12  | 2.17                     | 0.45              |
| 2:b:5317:ASN:O     | 2:b:5319:PRO:HD3   | 2.16                     | 0.45              |
| 2:b:5340:TRP:CZ3   | 2:b:5342:GLY:HA2   | 2.51                     | 0.45              |
| 22:b:6022:CLA:H143 | 22:b:6022:CLA:H71  | 1.94                     | 0.45              |
| 3:c:5139:THR:HG23  | 3:c:5142:GLU:HG3   | 1.98                     | 0.45              |
| 3:c:5404:LEU:C     | 3:c:5406:SER:N     | 2.73                     | 0.45              |
| 6:f:5024:HIS:O     | 6:f:5025:THR:C     | 2.59                     | 0.45              |
| 6:f:5037:ILE:HG22  | 9:j:5028:PHE:HE1   | 1.81                     | 0.45              |
| 7:h:5004:ARG:O     | 7:h:5005:THR:CG2   | 2.60                     | 0.45              |
| 12:m:5029:THR:C    | 12:m:5031:SER:H    | 2.24                     | 0.45              |
| 1:A:199:GLN:HE21   | 1:A:199:GLN:HB3    | 1.47                     | 0.45              |
| 26:A:1063:LHG:C32  | 22:K:1034:CLA:C15  | 2.87                     | 0.45              |
| 2:B:55:MET:CE      | 2:B:80:ILE:CG2     | 2.93                     | 0.45              |
| 2:B:271:THR:HG23   | 2:B:271:THR:O      | 2.16                     | 0.45              |
| 22:B:1010:CLA:CMD  | 22:B:1011:CLA:H92  | 2.46                     | 0.45              |
| 22:B:1012:CLA:HMD2 | 22:B:1020:CLA:H201 | 1.92                     | 0.45              |
| 22:B:1015:CLA:H141 | 22:B:1015:CLA:H161 | 1.77                     | 0.45              |
| 28:B:1060:MGE:H5B2 | 4:D:276:VAL:CB     | 2.46                     | 0.45              |
| 3:C:167:VAL:CG1    | 3:C:168:LEU:HD12   | 2.30                     | 0.45              |
| 3:C:320:ARG:O      | 3:C:324:LEU:HB2    | 2.17                     | 0.45              |
| 3:C:321:ASP:C      | 3:C:324:LEU:H      | 2.23                     | 0.45              |
| 3:C:371:GLY:N      | 3:C:374:GLY:O      | 2.49                     | 0.45              |
| 22:C:1025:CLA:C3A  | 22:C:1025:CLA:CGA  | 2.90                     | 0.45              |
| 22:C:1027:CLA:HHC  | 22:C:1027:CLA:HBB1 | 1.98                     | 0.45              |
| 22:C:1035:CLA:CBB  | 22:K:1034:CLA:CMA  | 2.91                     | 0.45              |
| 22:C:1035:CLA:H61  | 25:C:1052:BCR:H401 | 1.99                     | 0.45              |
| 4:D:275:PRO:O      | 4:D:278:GLY:N      | 2.50                     | 0.45              |
| 4:D:326:ARG:HG3    | 4:D:326:ARG:NH1    | 2.32                     | 0.45              |
| 22:D:1005:CLA:HBA2 | 22:D:1005:CLA:H3A  | 1.44                     | 0.45              |
| 25:H:1049:BCR:HC8  | 25:H:1049:BCR:C32  | 2.40                     | 0.45              |
| 22:K:1034:CLA:H91  | 22:K:1034:CLA:C12  | 2.44                     | 0.45              |
| 13:O:52:ALA:O      | 13:O:53:ARG:HB3    | 2.15                     | 0.45              |
| 13:O:59:ASP:HB3    | 13:O:61:SER:H      | 1.82                     | 0.45              |
| 13:O:97:VAL:HB     | 13:O:133:THR:O     | 2.17                     | 0.45              |
| 25:T:6046:BCR:C35  | 25:b:6047:BCR:C23  | 2.95                     | 0.45              |
| 15:U:36:ILE:O      | 15:U:38:TYR:N      | 2.46                     | 0.45              |
| 20:Z:26:ALA:CB     | 20:Z:40:ILE:HD11   | 2.47                     | 0.45              |
| 24:a:6043:PQ9:H401 | 24:a:6043:PQ9:H361 | 1.70                     | 0.45              |
| 2:b:5165:GLY:HA3   | 2:b:5179:GLN:C     | 2.42                     | 0.45              |
| 22:b:6015:CLA:OBD  | 22:b:6015:CLA:CED  | 2.38                     | 0.45              |
| 3:c:5143:TYR:O     | 3:c:5144:SER:C     | 2.59                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5171:GLY:CA    | 22:c:6025:CLA:CB   | 2.93                     | 0.45              |
| 22:c:6026:CLA:H2   | 22:c:6026:CLA:H62  | 1.63                     | 0.45              |
| 22:c:6032:CLA:HBC2 | 22:c:6032:CLA:CHD  | 2.47                     | 0.45              |
| 4:d:5180:ARG:NH1   | 4:d:5184:PHE:CD1   | 2.85                     | 0.45              |
| 4:d:5201:VAL:HG23  | 22:d:6004:CLA:CMB  | 2.20                     | 0.45              |
| 4:d:5269:PHE:C     | 4:d:5271:MET:N     | 2.72                     | 0.45              |
| 4:d:5275:PRO:O     | 4:d:5278:GLY:N     | 2.50                     | 0.45              |
| 24:d:6042:PQ9:C39  | 24:d:6042:PQ9:C42  | 2.36                     | 0.45              |
| 24:d:6042:PQ9:H211 | 24:d:6042:PQ9:H251 | 1.71                     | 0.45              |
| 25:d:6050:BCR:H331 | 25:d:6050:BCR:C8   | 2.28                     | 0.45              |
| 5:e:5068:ASP:H     | 5:e:5075:GLN:HE21  | 1.65                     | 0.45              |
| 10:k:5019:ASP:O    | 10:k:5023:ASP:OD1  | 2.33                     | 0.45              |
| 10:k:5033:PHE:H    | 22:k:6034:CLA:HMA3 | 1.81                     | 0.45              |
| 13:o:5185:PRO:O    | 13:o:5186:LYS:HB3  | 2.17                     | 0.45              |
| 13:o:5252:GLY:O    | 13:o:5253:ALA:C    | 2.59                     | 0.45              |
| 14:t:5011:ALA:C    | 14:t:5013:ILE:N    | 2.74                     | 0.45              |
| 15:u:5037:GLN:O    | 15:u:5038:TYR:CD2  | 2.70                     | 0.45              |
| 15:u:5088:GLU:HB3  | 15:u:5091:LEU:HB2  | 1.99                     | 0.45              |
| 1:A:20:TRP:O       | 1:A:21:VAL:C       | 2.59                     | 0.45              |
| 1:A:127:MET:C      | 1:A:130:GLN:HB3    | 2.42                     | 0.45              |
| 1:A:151:LEU:CD2    | 29:C:1055:DGD:HBS2 | 2.46                     | 0.45              |
| 1:A:265:PHE:HD1    | 1:A:271:LEU:CB     | 2.30                     | 0.45              |
| 1:A:272:HIS:HB3    | 4:D:218:VAL:HG11   | 1.97                     | 0.45              |
| 2:B:88:PRO:HB2     | 2:B:92:SER:HB2     | 1.99                     | 0.45              |
| 2:B:165:GLY:HA3    | 2:B:179:GLN:C      | 2.42                     | 0.45              |
| 2:B:241:SER:O      | 2:B:242:ILE:C      | 2.60                     | 0.45              |
| 2:B:290:ALA:O      | 2:B:294:SER:HB2    | 2.16                     | 0.45              |
| 3:C:33:PHE:CD2     | 4:D:229:ALA:HB1    | 2.51                     | 0.45              |
| 3:C:296:VAL:HG23   | 3:C:297:TYR:CE1    | 2.51                     | 0.45              |
| 3:C:461:ARG:HE     | 4:D:223:PHE:HD2    | 1.64                     | 0.45              |
| 4:D:15:PHE:CE1     | 4:D:32:TRP:CZ2     | 2.98                     | 0.45              |
| 4:D:273:PHE:C      | 4:D:273:PHE:CD2    | 2.95                     | 0.45              |
| 4:D:308:ASP:O      | 4:D:310:GLU:N      | 2.50                     | 0.45              |
| 24:D:1042:PQ9:C39  | 24:D:1042:PQ9:C42  | 2.36                     | 0.45              |
| 5:E:13:ILE:HG21    | 31:F:1040:HEM:CB   | 2.47                     | 0.45              |
| 12:M:34:LYS:HE2    | 11:l:5009:PRO:CB   | 2.45                     | 0.45              |
| 14:T:9:ILE:O       | 14:T:10:PHE:C      | 2.59                     | 0.45              |
| 1:a:5055:ALA:H     | 1:a:5070:SER:CB    | 2.30                     | 0.45              |
| 1:a:5104:GLU:OE1   | 13:o:5099:ARG:CD   | 2.65                     | 0.45              |
| 1:a:5252:HIS:CD2   | 1:a:5264:SER:HB3   | 2.51                     | 0.45              |
| 1:a:5258:LEU:O     | 1:a:5259:ILE:CG1   | 2.64                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5308:ASP:HB2   | 5:e:5052:PRO:O     | 2.17                     | 0.45              |
| 2:b:5021:ALA:HB2   | 2:b:5114:HIS:CB    | 2.46                     | 0.45              |
| 2:b:5033:TRP:HA    | 2:b:5036:SER:HB2   | 1.99                     | 0.45              |
| 2:b:5121:GLU:HB2   | 7:h:5004:ARG:CB    | 2.44                     | 0.45              |
| 2:b:5139:PHE:O     | 2:b:5140:GLY:C     | 2.60                     | 0.45              |
| 2:b:5271:THR:HG22  | 2:b:5274:GLN:CD    | 2.41                     | 0.45              |
| 2:b:5271:THR:HG23  | 2:b:5271:THR:O     | 2.16                     | 0.45              |
| 2:b:5460:LEU:HG    | 29:b:6058:DGD:CIA  | 2.47                     | 0.45              |
| 2:b:5482:ILE:O     | 2:b:5483:ASP:CB    | 2.62                     | 0.45              |
| 3:c:5293:ASN:HD22  | 3:c:5296:VAL:HG22  | 1.82                     | 0.45              |
| 3:c:5386:PRO:C     | 3:c:5388:GLN:N     | 2.73                     | 0.45              |
| 22:c:6028:CLA:H91  | 29:c:6056:DGD:C9B  | 2.47                     | 0.45              |
| 4:d:5014:TRP:O     | 4:d:5017:ILE:HG13  | 2.16                     | 0.45              |
| 4:d:5185:PHE:CD1   | 4:d:5289:LEU:HD13  | 2.52                     | 0.45              |
| 22:d:6004:CLA:H111 | 22:d:6004:CLA:H71  | 1.71                     | 0.45              |
| 25:d:6050:BCR:C21  | 28:d:6059:MGE:H3A2 | 2.47                     | 0.45              |
| 10:k:5043:VAL:O    | 10:k:5043:VAL:CG1  | 2.64                     | 0.45              |
| 11:l:5015:THR:O    | 11:l:5016:SER:C    | 2.60                     | 0.45              |
| 13:o:5145:LEU:O    | 13:o:5146:PHE:C    | 2.59                     | 0.45              |
| 15:u:5083:THR:CG2  | 15:u:5084:VAL:N    | 2.80                     | 0.45              |
| 17:x:5044:ASP:O    | 17:x:5044:ASP:OD1  | 2.34                     | 0.45              |
| 20:z:5016:SER:HA   | 20:z:5019:MET:HB2  | 1.97                     | 0.45              |
| 1:A:81:ALA:HB2     | 1:A:175:GLY:HA3    | 1.98                     | 0.45              |
| 1:A:204:GLY:O      | 1:A:205:VAL:C      | 2.58                     | 0.45              |
| 2:B:185:TRP:CD1    | 2:B:185:TRP:H      | 2.33                     | 0.45              |
| 2:B:340:TRP:CZ3    | 2:B:342:GLY:HA2    | 2.51                     | 0.45              |
| 3:C:53:HIS:O       | 3:C:57:ALA:HB2     | 2.17                     | 0.45              |
| 3:C:69:LEU:O       | 3:C:73:ALA:HB2     | 2.17                     | 0.45              |
| 3:C:223:TRP:CD1    | 3:C:224:ILE:HD13   | 2.51                     | 0.45              |
| 4:D:114:ILE:CG2    | 23:D:1039:PHO:H121 | 2.47                     | 0.45              |
| 4:D:217:THR:HG23   | 4:D:218:VAL:N      | 2.32                     | 0.45              |
| 7:H:30:LEU:HA      | 7:H:33:VAL:CG2     | 2.47                     | 0.45              |
| 13:O:45:CYS:CB     | 13:O:46:PRO:HD2    | 2.32                     | 0.45              |
| 13:O:185:PRO:O     | 13:O:186:LYS:HB3   | 2.17                     | 0.45              |
| 15:U:32:ILE:HG13   | 15:U:50:VAL:HG21   | 1.98                     | 0.45              |
| 15:U:37:GLN:O      | 15:U:38:TYR:CD2    | 2.70                     | 0.45              |
| 15:U:73:GLN:O      | 15:U:74:ILE:C      | 2.59                     | 0.45              |
| 19:N:2:UNK:O       | 19:N:3:UNK:C       | 2.65                     | 0.45              |
| 1:a:5259:ILE:CD1   | 24:a:6043:PQ9:H242 | 2.37                     | 0.45              |
| 2:b:5012:LEU:HD23  | 2:b:5019:LEU:HA    | 1.99                     | 0.45              |
| 2:b:5025:MET:HE3   | 2:b:5025:MET:HB3   | 1.79                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5088:PRO:HB2   | 2:b:5092:SER:HB2   | 1.99                     | 0.45              |
| 2:b:5121:GLU:O     | 2:b:5124:ARG:N     | 2.35                     | 0.45              |
| 2:b:5224:ARG:HG2   | 7:h:5025:TRP:CD1   | 2.51                     | 0.45              |
| 2:b:5237:VAL:HB    | 22:b:6020:CLA:HMD2 | 1.99                     | 0.45              |
| 3:c:5128:GLY:HA3   | 22:c:6037:CLA:C3C  | 2.46                     | 0.45              |
| 3:c:5206:PRO:O     | 3:c:5210:PHE:HB2   | 2.16                     | 0.45              |
| 3:c:5340:TYR:CD2   | 3:c:5340:TYR:N     | 2.71                     | 0.45              |
| 3:c:5431:PHE:CD2   | 3:c:5431:PHE:O     | 2.69                     | 0.45              |
| 22:c:6026:CLA:HBB2 | 22:k:6034:CLA:H11  | 1.98                     | 0.45              |
| 4:d:5261:PHE:HE2   | 4:d:5266:TRP:CD1   | 2.35                     | 0.45              |
| 5:e:5010:PHE:CE1   | 6:f:5019:ARG:HD2   | 2.52                     | 0.45              |
| 5:e:5037:PHE:CZ    | 5:e:5046:VAL:HG21  | 2.52                     | 0.45              |
| 8:i:5004:LEU:HA    | 8:i:5004:LEU:HD12  | 1.79                     | 0.45              |
| 22:k:6034:CLA:CHD  | 22:k:6034:CLA:CBC  | 2.84                     | 0.45              |
| 13:o:5163:THR:OG1  | 13:o:5164:THR:N    | 2.50                     | 0.45              |
| 13:o:5235:GLY:HA3  | 13:o:5269:ILE:O    | 2.17                     | 0.45              |
| 15:u:5042:TYR:HD2  | 15:u:5043:PRO:N    | 2.12                     | 0.45              |
| 15:u:5057:SER:OG   | 15:u:5060:ASP:OD2  | 2.34                     | 0.45              |
| 16:v:5090:PRO:HD2  | 16:v:5092:ARG:NH1  | 2.32                     | 0.45              |
| 18:y:5043:ARG:CZ   | 18:y:5043:ARG:H    | 2.30                     | 0.45              |
| 1:A:119:PHE:O      | 1:A:121:LEU:N      | 2.50                     | 0.44              |
| 2:B:46:ASP:N       | 2:B:58:GLN:HE22    | 2.15                     | 0.44              |
| 2:B:67:ALA:O       | 2:B:68:ARG:C       | 2.60                     | 0.44              |
| 2:B:249:ALA:C      | 2:B:251:VAL:N      | 2.75                     | 0.44              |
| 2:B:460:LEU:HG     | 29:B:1058:DGD:CIA  | 2.47                     | 0.44              |
| 22:B:1015:CLA:CBB  | 22:B:1015:CLA:HHC  | 2.46                     | 0.44              |
| 25:B:1048:BCR:C40  | 25:B:1048:BCR:H372 | 2.29                     | 0.44              |
| 3:C:318:LEU:CD2    | 3:C:318:LEU:C      | 2.90                     | 0.44              |
| 22:C:1036:CLA:CMC  | 22:C:1036:CLA:CBC  | 2.95                     | 0.44              |
| 22:C:1036:CLA:H162 | 22:C:1036:CLA:H122 | 1.60                     | 0.44              |
| 22:D:1005:CLA:H203 | 22:D:1005:CLA:H161 | 1.75                     | 0.44              |
| 25:D:1050:BCR:C21  | 28:D:1059:MGE:H3A2 | 2.47                     | 0.44              |
| 9:J:24:ILE:CG2     | 9:J:25:VAL:N       | 2.80                     | 0.44              |
| 13:O:47:THR:O      | 13:O:48:LEU:HD23   | 2.16                     | 0.44              |
| 13:O:151:LEU:HG    | 13:O:152:VAL:N     | 2.31                     | 0.44              |
| 13:O:163:THR:OG1   | 13:O:164:THR:N     | 2.50                     | 0.44              |
| 15:U:26:ASP:C      | 15:U:26:ASP:OD1    | 2.60                     | 0.44              |
| 15:U:57:SER:OG     | 15:U:60:ASP:OD2    | 2.34                     | 0.44              |
| 18:Y:21:GLN:O      | 18:Y:25:ILE:CG2    | 2.65                     | 0.44              |
| 1:a:5119:PHE:CZ    | 22:a:6003:CLA:H102 | 2.52                     | 0.44              |
| 1:a:5161:TYR:CZ    | 1:a:5186:PHE:CE2   | 3.06                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5320:ILE:O     | 1:a:5323:ARG:N     | 2.50                     | 0.44              |
| 2:b:5018:ARG:HH21  | 2:b:5115:TRP:NE1   | 2.16                     | 0.44              |
| 2:b:5089:GLY:O     | 2:b:5090:PHE:C     | 2.59                     | 0.44              |
| 2:b:5168:VAL:HG12  | 2:b:5169:SER:H     | 1.80                     | 0.44              |
| 3:c:5337:LEU:HD22  | 3:c:5342:MET:HG3   | 1.99                     | 0.44              |
| 4:d:5014:TRP:CD1   | 4:d:5014:TRP:C     | 2.91                     | 0.44              |
| 4:d:5053:THR:HG23  | 4:d:5067:TYR:CD2   | 2.52                     | 0.44              |
| 4:d:5103:ARG:HG3   | 5:e:5073:LYS:HD3   | 1.97                     | 0.44              |
| 4:d:5189:HIS:ND1   | 4:d:5294:ARG:HD3   | 2.31                     | 0.44              |
| 5:e:5013:ILE:HG21  | 31:f:6040:HEM:CBC  | 2.47                     | 0.44              |
| 9:j:5029:PHE:O     | 9:j:5030:TYR:C     | 2.60                     | 0.44              |
| 13:o:5059:ASP:CB   | 13:o:5062:GLN:HB2  | 2.47                     | 0.44              |
| 13:o:5059:ASP:HB3  | 13:o:5061:SER:H    | 1.82                     | 0.44              |
| 13:o:5079:LYS:CE   | 13:o:5089:ALA:HB3  | 2.47                     | 0.44              |
| 13:o:5097:VAL:HB   | 13:o:5133:THR:O    | 2.17                     | 0.44              |
| 13:o:5184:ASP:OD2  | 13:o:5188:ARG:NH1  | 2.50                     | 0.44              |
| 13:o:5265:PHE:CD1  | 13:o:5265:PHE:C    | 2.94                     | 0.44              |
| 15:u:5024:LYS:HB3  | 15:u:5081:HIS:O    | 2.17                     | 0.44              |
| 15:u:5026:ASP:C    | 15:u:5026:ASP:OD1  | 2.60                     | 0.44              |
| 15:u:5043:PRO:HG3  | 16:v:5109:ASP:HA   | 1.97                     | 0.44              |
| 19:n:5002:UNK:O    | 19:n:5003:UNK:C    | 2.65                     | 0.44              |
| 1:A:27:ARG:HG3     | 1:A:27:ARG:NH1     | 2.33                     | 0.44              |
| 1:A:38:ILE:HG22    | 1:A:39:PRO:CD      | 2.46                     | 0.44              |
| 1:A:145:VAL:O      | 1:A:146:ALA:C      | 2.59                     | 0.44              |
| 1:A:193:LEU:HD22   | 4:D:179:PHE:CG     | 2.52                     | 0.44              |
| 22:A:1007:CLA:C6   | 22:A:1007:CLA:C11  | 2.92                     | 0.44              |
| 2:B:121:GLU:HB2    | 7:H:4:ARG:CB       | 2.44                     | 0.44              |
| 2:B:139:PHE:O      | 2:B:140:GLY:C      | 2.60                     | 0.44              |
| 2:B:272:ARG:HA     | 2:B:319:PRO:HD2    | 1.99                     | 0.44              |
| 2:B:477:ASP:OD2    | 4:D:134:ARG:NH1    | 2.43                     | 0.44              |
| 3:C:62:PHE:HE2     | 10:K:29:PRO:CD     | 2.30                     | 0.44              |
| 3:C:139:THR:HG23   | 3:C:142:GLU:HG3    | 1.98                     | 0.44              |
| 3:C:210:PHE:HE1    | 3:C:239:TRP:CE3    | 2.35                     | 0.44              |
| 3:C:225:VAL:HG23   | 3:C:226:SER:H      | 1.80                     | 0.44              |
| 22:C:1028:CLA:H93  | 29:C:1056:DGD:HB91 | 1.97                     | 0.44              |
| 22:C:1033:CLA:HMA3 | 22:K:1034:CLA:CAC  | 2.42                     | 0.44              |
| 22:C:1035:CLA:CMB  | 25:C:1052:BCR:H271 | 2.46                     | 0.44              |
| 29:C:1057:DGD:HAS2 | 28:D:1059:MGE:CDB  | 2.47                     | 0.44              |
| 4:D:79:SER:C       | 4:D:80:THR:HG22    | 2.42                     | 0.44              |
| 4:D:161:PRO:CG     | 4:D:170:ALA:HB2    | 2.47                     | 0.44              |
| 4:D:297:ASP:O      | 4:D:298:PHE:HB2    | 2.15                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:308:ASP:OD1    | 4:D:310:GLU:HG2    | 2.17                     | 0.44              |
| 13:O:48:LEU:HD12   | 13:O:229:LYS:O     | 2.17                     | 0.44              |
| 14:T:4:ILE:O       | 14:T:8:PHE:N       | 2.48                     | 0.44              |
| 15:U:24:LYS:HB3    | 15:U:81:HIS:O      | 2.17                     | 0.44              |
| 16:V:90:PRO:HD2    | 16:V:92:ARG:NH1    | 2.32                     | 0.44              |
| 18:Y:43:ARG:CD     | 20:Z:29:SER:HA     | 2.46                     | 0.44              |
| 1:a:5027:ARG:HG3   | 1:a:5027:ARG:NH1   | 2.32                     | 0.44              |
| 1:a:5193:LEU:HD22  | 4:d:5179:PHE:CG    | 2.52                     | 0.44              |
| 1:a:5288:LEU:HD22  | 3:c:5432:VAL:HA    | 1.98                     | 0.44              |
| 1:a:5318:ALA:HA    | 1:a:5321:ILE:HD12  | 1.99                     | 0.44              |
| 1:a:5337:HIS:O     | 4:d:5350:ASN:O     | 2.35                     | 0.44              |
| 2:b:5063:LEU:N     | 2:b:5064:PRO:HD3   | 2.33                     | 0.44              |
| 2:b:5074:SER:HA    | 2:b:5092:SER:OG    | 2.16                     | 0.44              |
| 2:b:5231:MET:HG2   | 22:b:6018:CLA:HAC2 | 1.98                     | 0.44              |
| 2:b:5249:ALA:C     | 2:b:5251:VAL:N     | 2.75                     | 0.44              |
| 28:b:6060:MGE:H5B2 | 4:d:5276:VAL:CB    | 2.46                     | 0.44              |
| 22:c:6028:CLA:H202 | 22:c:6028:CLA:H161 | 1.61                     | 0.44              |
| 22:c:6029:CLA:H11  | 22:c:6029:CLA:C1A  | 2.47                     | 0.44              |
| 22:c:6031:CLA:H142 | 22:c:6031:CLA:H111 | 1.75                     | 0.44              |
| 22:c:6036:CLA:CMC  | 22:c:6036:CLA:CBC  | 2.95                     | 0.44              |
| 4:d:5016:ASP:O     | 4:d:5020:ASP:HB2   | 2.18                     | 0.44              |
| 5:e:5024:SER:O     | 5:e:5028:PRO:HD2   | 2.17                     | 0.44              |
| 5:e:5047:PHE:C     | 5:e:5049:THR:N     | 2.74                     | 0.44              |
| 12:m:5027:VAL:O    | 12:m:5027:VAL:HG12 | 2.18                     | 0.44              |
| 13:o:5210:ARG:NE   | 13:o:5252:GLY:O    | 2.49                     | 0.44              |
| 17:x:5011:THR:O    | 17:x:5011:THR:CG2  | 2.65                     | 0.44              |
| 20:z:5004:LEU:HD12 | 20:z:5004:LEU:O    | 2.17                     | 0.44              |
| 1:A:276:ALA:O      | 1:A:280:VAL:HG23   | 2.17                     | 0.44              |
| 1:A:320:ILE:HD13   | 1:A:320:ILE:HA     | 1.91                     | 0.44              |
| 2:B:15:ASP:N       | 2:B:16:PRO:CD      | 2.79                     | 0.44              |
| 2:B:341:LYS:HD2    | 2:B:429:ILE:HG22   | 2.00                     | 0.44              |
| 3:C:53:HIS:HB2     | 22:C:1036:CLA:HMD2 | 1.98                     | 0.44              |
| 3:C:78:GLU:H       | 3:C:78:GLU:CD      | 2.26                     | 0.44              |
| 3:C:223:TRP:HD1    | 3:C:224:ILE:N      | 2.13                     | 0.44              |
| 3:C:455:PHE:O      | 3:C:458:GLY:O      | 2.35                     | 0.44              |
| 22:C:1035:CLA:HHC  | 22:C:1035:CLA:CBB  | 2.20                     | 0.44              |
| 4:D:27:PHE:CD1     | 6:F:19:ARG:HG3     | 2.52                     | 0.44              |
| 4:D:249:ALA:O      | 4:D:252:PHE:N      | 2.41                     | 0.44              |
| 4:D:258:GLY:C      | 4:D:259:ILE:HD13   | 2.40                     | 0.44              |
| 5:E:37:PHE:CZ      | 5:E:46:VAL:HG21    | 2.52                     | 0.44              |
| 13:O:59:ASP:CB     | 13:O:62:GLN:HB2    | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:U:61:VAL:HG12   | 15:U:75:LEU:CD2    | 2.37                     | 0.44              |
| 16:V:103:LYS:CD    | 16:V:121:LEU:HD12  | 2.28                     | 0.44              |
| 1:a:5093:PHE:CB    | 3:c:5218:PHE:HD2   | 2.27                     | 0.44              |
| 1:a:5328:MET:HE2   | 4:d:5183:LEU:HD13  | 1.98                     | 0.44              |
| 1:a:5333:GLU:CB    | 1:a:5337:HIS:CE1   | 3.01                     | 0.44              |
| 23:a:6038:PHO:C4   | 23:a:6038:PHO:C7   | 2.93                     | 0.44              |
| 23:a:6038:PHO:CED  | 23:a:6038:PHO:OBD  | 2.66                     | 0.44              |
| 2:b:5069:LEU:CD2   | 22:b:6013:CLA:O1A  | 2.64                     | 0.44              |
| 2:b:5357:ARG:HH11  | 2:b:5357:ARG:CG    | 2.26                     | 0.44              |
| 2:b:5367:PRO:O     | 2:b:5367:PRO:HG2   | 2.18                     | 0.44              |
| 22:b:6012:CLA:H12  | 22:b:6013:CLA:C4   | 2.37                     | 0.44              |
| 22:b:6016:CLA:H202 | 22:d:6008:CLA:HAA2 | 2.00                     | 0.44              |
| 3:c:5069:LEU:O     | 3:c:5073:ALA:HB2   | 2.17                     | 0.44              |
| 3:c:5078:GLU:H     | 3:c:5078:GLU:CD    | 2.26                     | 0.44              |
| 3:c:5081:MET:SD    | 3:c:5090:PRO:HA    | 2.57                     | 0.44              |
| 3:c:5318:LEU:CD2   | 3:c:5318:LEU:C     | 2.90                     | 0.44              |
| 22:c:6027:CLA:HHC  | 22:c:6027:CLA:CBB  | 2.48                     | 0.44              |
| 22:c:6031:CLA:CMD  | 22:c:6033:CLA:H162 | 2.48                     | 0.44              |
| 4:d:5103:ARG:O     | 4:d:5106:GLN:N     | 2.48                     | 0.44              |
| 4:d:5273:PHE:CD2   | 4:d:5273:PHE:C     | 2.95                     | 0.44              |
| 4:d:5308:ASP:OD1   | 4:d:5310:GLU:HG2   | 2.18                     | 0.44              |
| 25:h:6049:BCR:C40  | 17:x:5020:PHE:HZ   | 2.28                     | 0.44              |
| 15:u:5068:THR:HG22 | 15:u:5071:GLN:CG   | 2.48                     | 0.44              |
| 16:v:5088:ALA:HA   | 16:v:5108:TYR:CD2  | 2.48                     | 0.44              |
| 18:y:5043:ARG:CD   | 20:z:5029:SER:HA   | 2.47                     | 0.44              |
| 1:A:55:ALA:H       | 1:A:70:SER:CB      | 2.30                     | 0.44              |
| 1:A:104:GLU:OE1    | 13:O:99:ARG:CD     | 2.65                     | 0.44              |
| 1:A:215:HIS:ND1    | 24:A:1043:PQ9:O1   | 2.51                     | 0.44              |
| 1:A:286:ALA:O      | 1:A:289:GLY:N      | 2.51                     | 0.44              |
| 2:B:136:PRO:HB3    | 2:B:221:PRO:HG3    | 2.00                     | 0.44              |
| 2:B:237:VAL:HB     | 22:B:1020:CLA:CMD  | 2.48                     | 0.44              |
| 2:B:323:GLY:C      | 4:D:293:LEU:HD23   | 2.43                     | 0.44              |
| 22:B:1012:CLA:CHD  | 22:B:1020:CLA:C20  | 2.94                     | 0.44              |
| 25:B:1047:BCR:C23  | 25:t:1046:BCR:C35  | 2.95                     | 0.44              |
| 3:C:79:LYS:HB3     | 3:C:84:GLN:CD      | 2.39                     | 0.44              |
| 3:C:89:ILE:O       | 3:C:111:PHE:HE2    | 2.00                     | 0.44              |
| 3:C:385:GLN:HB3    | 3:C:386:PRO:CD     | 2.48                     | 0.44              |
| 22:C:1028:CLA:H91  | 29:C:1056:DGD:C9B  | 2.47                     | 0.44              |
| 22:C:1033:CLA:H3A  | 22:C:1033:CLA:HBA1 | 1.75                     | 0.44              |
| 4:D:247:VAL:C      | 4:D:249:ALA:H      | 2.26                     | 0.44              |
| 4:D:262:SER:N      | 28:D:1062:MGE:O3D  | 2.51                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:I:6:ILE:O        | 8:I:10:ILE:HD11    | 2.17                     | 0.44              |
| 8:I:25:SER:O       | 8:I:26:GLY:O       | 2.36                     | 0.44              |
| 13:O:64:TYR:HA     | 13:O:271:PRO:HA    | 1.99                     | 0.44              |
| 15:U:29:ASN:O      | 15:U:30:THR:C      | 2.60                     | 0.44              |
| 15:U:68:THR:HG22   | 15:U:71:GLN:CG     | 2.48                     | 0.44              |
| 1:a:5160:ILE:O     | 1:a:5161:TYR:C     | 2.60                     | 0.44              |
| 2:b:5061:PHE:HB2   | 22:b:6015:CLA:CMA  | 2.48                     | 0.44              |
| 22:b:6009:CLA:H141 | 22:b:6009:CLA:H162 | 1.64                     | 0.44              |
| 22:b:6015:CLA:H71  | 22:b:6015:CLA:H42  | 1.94                     | 0.44              |
| 22:b:6020:CLA:H112 | 22:b:6020:CLA:H91  | 1.56                     | 0.44              |
| 3:c:5053:HIS:HB2   | 22:c:6036:CLA:HMD2 | 1.98                     | 0.44              |
| 29:c:6057:DGD:O2D  | 9:j:5032:ALA:HB1   | 2.18                     | 0.44              |
| 4:d:5049:LEU:HD13  | 25:d:6050:BCR:C14  | 2.47                     | 0.44              |
| 4:d:5109:GLY:C     | 4:d:5111:TRP:H     | 2.25                     | 0.44              |
| 4:d:5161:PRO:CG    | 4:d:5170:ALA:HB2   | 2.47                     | 0.44              |
| 4:d:5253:TRP:O     | 4:d:5254:SER:C     | 2.61                     | 0.44              |
| 4:d:5262:SER:N     | 28:d:6062:MGE:O3D  | 2.51                     | 0.44              |
| 4:d:5270:PHE:CD1   | 4:d:5270:PHE:O     | 2.70                     | 0.44              |
| 4:d:5337:GLU:HG2   | 4:d:5339:PHE:CZ    | 2.53                     | 0.44              |
| 13:o:5070:CYS:HB2  | 13:o:5105:ASP:CB   | 2.47                     | 0.44              |
| 14:t:5010:PHE:C    | 14:t:5010:PHE:CD1  | 2.95                     | 0.44              |
| 1:A:20:TRP:CD1     | 1:A:26:ASN:HD21    | 2.35                     | 0.44              |
| 1:A:89:ILE:HD13    | 1:A:94:TYR:CG      | 2.53                     | 0.44              |
| 1:A:132:GLU:O      | 1:A:136:ARG:HG2    | 2.17                     | 0.44              |
| 2:B:35:GLY:O       | 2:B:39:LEU:HG      | 2.18                     | 0.44              |
| 2:B:153:PHE:HD1    | 2:B:157:HIS:CB     | 2.30                     | 0.44              |
| 2:B:191:ASN:HD21   | 7:H:60:VAL:CA      | 2.19                     | 0.44              |
| 2:B:196:GLY:C      | 2:B:198:VAL:N      | 2.74                     | 0.44              |
| 22:B:1010:CLA:C2D  | 22:B:1011:CLA:HMB1 | 2.48                     | 0.44              |
| 3:C:70:PHE:O       | 3:C:74:HIS:ND1     | 2.47                     | 0.44              |
| 3:C:330:SER:HB2    | 13:O:126:GLY:O     | 2.17                     | 0.44              |
| 22:C:1025:CLA:CHB  | 22:C:1025:CLA:O2A  | 2.60                     | 0.44              |
| 25:C:1052:BCR:H403 | 25:C:1052:BCR:H24C | 1.76                     | 0.44              |
| 8:I:24:LEU:C       | 8:I:26:GLY:N       | 2.70                     | 0.44              |
| 13:O:65:ARG:HG2    | 13:O:66:ILE:N      | 2.33                     | 0.44              |
| 13:O:172:PHE:HD1   | 13:O:221:GLY:HA3   | 1.77                     | 0.44              |
| 13:O:235:GLY:HA3   | 13:O:269:ILE:O     | 2.17                     | 0.44              |
| 22:a:6006:CLA:H2   | 22:a:6006:CLA:H61  | 1.67                     | 0.44              |
| 23:a:6038:PHO:H161 | 23:a:6038:PHO:H143 | 1.62                     | 0.44              |
| 2:b:5101:ILE:O     | 25:b:6047:BCR:H391 | 2.17                     | 0.44              |
| 2:b:5460:LEU:CA    | 29:b:6058:DGD:HAG1 | 2.38                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5062:PHE:HE2   | 10:k:5029:PRO:CD   | 2.30                     | 0.44              |
| 24:d:6042:PQ9:C40  | 11:l:5030:LEU:HD12 | 2.38                     | 0.44              |
| 7:h:5030:LEU:HA    | 7:h:5033:VAL:CG2   | 2.48                     | 0.44              |
| 13:o:5160:THR:O    | 13:o:5160:THR:CG2  | 2.66                     | 0.44              |
| 13:o:5173:ASN:HD22 | 13:o:5173:ASN:HA   | 1.54                     | 0.44              |
| 1:A:121:LEU:O      | 1:A:124:SER:N      | 2.51                     | 0.44              |
| 1:A:309:ALA:HB3    | 16:V:28:GLU:CB     | 2.47                     | 0.44              |
| 1:A:328:MET:HE2    | 4:D:183:LEU:HD13   | 1.98                     | 0.44              |
| 24:A:1043:PQ9:H292 | 24:A:1043:PQ9:H393 | 1.99                     | 0.44              |
| 2:B:151:PHE:HB2    | 2:B:206:GLY:HA3    | 1.98                     | 0.44              |
| 2:B:488:PRO:O      | 2:B:489:GLU:CB     | 2.59                     | 0.44              |
| 22:B:1016:CLA:H202 | 22:D:1008:CLA:HAA2 | 2.00                     | 0.44              |
| 22:B:1019:CLA:H122 | 22:B:1019:CLA:H162 | 1.51                     | 0.44              |
| 22:B:1022:CLA:H152 | 12:M:24:ILE:HG21   | 1.99                     | 0.44              |
| 3:C:87:ILE:HG13    | 3:C:88:LEU:H       | 1.82                     | 0.44              |
| 3:C:257:PHE:HD1    | 3:C:257:PHE:N      | 2.09                     | 0.44              |
| 3:C:420:VAL:HG21   | 3:C:425:TRP:HZ2    | 1.83                     | 0.44              |
| 22:C:1028:CLA:H91  | 29:C:1056:DGD:HB91 | 1.98                     | 0.44              |
| 29:C:1057:DGD:HB72 | 28:D:1059:MGE:H7B1 | 1.99                     | 0.44              |
| 4:D:109:GLY:C      | 4:D:111:TRP:H      | 2.25                     | 0.44              |
| 4:D:145:ALA:HA     | 4:D:276:VAL:HG11   | 2.00                     | 0.44              |
| 4:D:217:THR:CG2    | 4:D:218:VAL:N      | 2.81                     | 0.44              |
| 4:D:265:ARG:NH1    | 4:D:265:ARG:CG     | 2.70                     | 0.44              |
| 22:D:1005:CLA:H91  | 28:D:1062:MGE:H263 | 1.99                     | 0.44              |
| 22:D:1008:CLA:H18  | 22:D:1008:CLA:H151 | 1.58                     | 0.44              |
| 8:I:27:ASP:C       | 8:I:29:ALA:N       | 2.73                     | 0.44              |
| 10:K:17:ILE:HB     | 10:K:18:PHE:CD1    | 2.53                     | 0.44              |
| 13:O:52:ALA:HB1    | 13:O:229:LYS:HA    | 2.00                     | 0.44              |
| 14:T:10:PHE:C      | 14:T:10:PHE:CD1    | 2.95                     | 0.44              |
| 25:T:6046:BCR:H341 | 25:b:6047:BCR:H272 | 1.99                     | 0.44              |
| 1:a:5119:PHE:O     | 1:a:5121:LEU:N     | 2.50                     | 0.44              |
| 1:a:5187:GLN:CG    | 1:a:5325:ASN:HD21  | 2.16                     | 0.44              |
| 1:a:5265:PHE:HD1   | 1:a:5271:LEU:CB    | 2.30                     | 0.44              |
| 2:b:5241:SER:O     | 2:b:5242:ILE:C     | 2.60                     | 0.44              |
| 22:b:6023:CLA:H151 | 22:b:6024:CLA:C4A  | 2.48                     | 0.44              |
| 3:c:5046:SER:OG    | 3:c:5141:GLU:CB    | 2.60                     | 0.44              |
| 3:c:5046:SER:OG    | 3:c:5141:GLU:CA    | 2.65                     | 0.44              |
| 3:c:5207:ARG:O     | 3:c:5211:GLY:HA3   | 2.17                     | 0.44              |
| 3:c:5431:PHE:C     | 3:c:5431:PHE:HD2   | 2.23                     | 0.44              |
| 22:c:6033:CLA:C15  | 22:c:6033:CLA:C20  | 2.95                     | 0.44              |
| 22:c:6035:CLA:HMC3 | 22:k:6034:CLA:CMB  | 2.48                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:d:5090:LEU:CD2   | 4:d:5109:GLY:H     | 2.31                     | 0.44              |
| 4:d:5100:ASP:C     | 4:d:5102:THR:H     | 2.25                     | 0.44              |
| 25:d:6050:BCR:C19  | 28:d:6059:MGE:H102 | 2.48                     | 0.44              |
| 8:i:5006:ILE:O     | 8:i:5010:ILE:HD11  | 2.17                     | 0.44              |
| 9:j:5024:ILE:CG2   | 9:j:5025:VAL:N     | 2.80                     | 0.44              |
| 13:o:5048:LEU:HD12 | 13:o:5229:LYS:O    | 2.17                     | 0.44              |
| 13:o:5052:ALA:HB1  | 13:o:5229:LYS:HA   | 2.00                     | 0.44              |
| 13:o:5065:ARG:HG2  | 13:o:5066:ILE:N    | 2.33                     | 0.44              |
| 13:o:5184:ASP:OD1  | 13:o:5188:ARG:HB2  | 2.18                     | 0.44              |
| 1:A:137:LEU:HB3    | 1:A:139:MET:HE3    | 2.00                     | 0.44              |
| 1:A:160:ILE:HD13   | 3:C:431:PHE:HE1    | 1.80                     | 0.44              |
| 1:A:160:ILE:O      | 1:A:161:TYR:C      | 2.60                     | 0.44              |
| 1:A:202:VAL:O      | 1:A:206:PHE:HB2    | 2.18                     | 0.44              |
| 1:A:215:HIS:CD2    | 1:A:275:LEU:CD1    | 3.00                     | 0.44              |
| 1:A:308:ASP:HB2    | 5:E:52:PRO:O       | 2.17                     | 0.44              |
| 2:B:18:ARG:HH21    | 2:B:115:TRP:NE1    | 2.16                     | 0.44              |
| 2:B:247:PHE:CE1    | 2:B:251:VAL:CG2    | 3.01                     | 0.44              |
| 2:B:331:ASN:C      | 2:B:333:GLY:N      | 2.76                     | 0.44              |
| 2:B:367:PRO:O      | 2:B:367:PRO:HG2    | 2.18                     | 0.44              |
| 3:C:39:ASN:CG      | 22:C:1033:CLA:HBB2 | 2.42                     | 0.44              |
| 3:C:143:TYR:CE2    | 22:C:1037:CLA:HED2 | 2.53                     | 0.44              |
| 3:C:223:TRP:HD1    | 3:C:224:ILE:HD13   | 1.83                     | 0.44              |
| 3:C:293:ASN:HD22   | 3:C:296:VAL:HG22   | 1.82                     | 0.44              |
| 3:C:457:LYS:HD2    | 4:D:224:GLN:NE2    | 2.33                     | 0.44              |
| 22:C:1035:CLA:H111 | 25:C:1052:BCR:H24C | 1.98                     | 0.44              |
| 4:D:85:MET:HA      | 5:E:69:ARG:HB3     | 2.00                     | 0.44              |
| 4:D:253:TRP:HD1    | 24:D:1042:PQ9:H92  | 1.82                     | 0.44              |
| 28:D:1062:MGE:H2G  | 28:D:1062:MGE:H1D  | 1.40                     | 0.44              |
| 13:O:59:ASP:O      | 13:O:60:SER:HB2    | 2.16                     | 0.44              |
| 13:O:92:VAL:HG12   | 13:O:93:PRO:HD2    | 2.00                     | 0.44              |
| 15:U:51:LYS:O      | 15:U:52:ASN:O      | 2.36                     | 0.44              |
| 31:V:1041:HEM:HHC  | 31:V:1041:HEM:HBB2 | 1.99                     | 0.44              |
| 1:a:5031:GLY:HA3   | 1:a:5132:GLU:CD    | 2.42                     | 0.44              |
| 1:a:5051:ALA:O     | 1:a:5055:ALA:HB3   | 2.18                     | 0.44              |
| 1:a:5151:LEU:CD2   | 29:c:6055:DGD:HBS2 | 2.46                     | 0.44              |
| 1:a:5202:VAL:O     | 1:a:5206:PHE:HB2   | 2.18                     | 0.44              |
| 2:b:5030:VAL:HG22  | 22:b:6021:CLA:C2C  | 2.48                     | 0.44              |
| 2:b:5046:ASP:N     | 2:b:5058:GLN:HE22  | 2.15                     | 0.44              |
| 2:b:5220:ARG:CD    | 7:h:5020:LYS:O     | 2.58                     | 0.44              |
| 22:b:6011:CLA:C2D  | 22:b:6013:CLA:H12  | 2.45                     | 0.44              |
| 3:c:5053:HIS:O     | 3:c:5057:ALA:HB2   | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5206:PRO:HG2   | 3:c:5207:ARG:HH11  | 1.81                     | 0.44              |
| 3:c:5239:TRP:HE3   | 3:c:5243:ILE:HD11  | 1.81                     | 0.44              |
| 3:c:5277:GLY:HA3   | 3:c:5441:HIS:HD2   | 1.81                     | 0.44              |
| 3:c:5440:GLY:O     | 3:c:5442:LEU:N     | 2.50                     | 0.44              |
| 3:c:5455:PHE:O     | 3:c:5458:GLY:O     | 2.35                     | 0.44              |
| 22:c:6025:CLA:C4   | 22:c:6025:CLA:HMB3 | 2.40                     | 0.44              |
| 22:c:6037:CLA:H142 | 22:c:6037:CLA:C10  | 2.48                     | 0.44              |
| 4:d:5103:ARG:HA    | 4:d:5106:GLN:HE21  | 1.83                     | 0.44              |
| 4:d:5114:ILE:CG2   | 23:d:6039:PHO:H121 | 2.47                     | 0.44              |
| 4:d:5155:SER:HA    | 4:d:5159:ILE:CG1   | 2.47                     | 0.44              |
| 4:d:5161:PRO:CG    | 4:d:5170:ALA:CB    | 2.96                     | 0.44              |
| 4:d:5347:PRO:C     | 4:d:5348:ARG:HG3   | 2.43                     | 0.44              |
| 10:k:5032:PHE:C    | 10:k:5034:ALA:N    | 2.74                     | 0.44              |
| 11:l:5024:ILE:CD1  | 12:m:5018:PRO:HB2  | 2.48                     | 0.44              |
| 13:o:5058:ILE:HG23 | 13:o:5160:THR:O    | 2.18                     | 0.44              |
| 13:o:5216:PHE:C    | 13:o:5216:PHE:CD2  | 2.94                     | 0.44              |
| 16:v:5090:PRO:HD2  | 16:v:5092:ARG:NH2  | 2.32                     | 0.44              |
| 31:v:6041:HEM:HBB2 | 31:v:6041:HEM:HHC  | 1.99                     | 0.44              |
| 1:A:310:LYS:HD3    | 1:A:312:ASN:ND2    | 2.33                     | 0.44              |
| 2:B:6:TYR:H        | 2:B:6:TYR:HD2      | 1.57                     | 0.44              |
| 2:B:30:VAL:HG22    | 22:B:1021:CLA:C2C  | 2.48                     | 0.44              |
| 2:B:168:VAL:HG12   | 2:B:169:SER:H      | 1.79                     | 0.44              |
| 2:B:264:PRO:HG3    | 2:B:267:LEU:HD12   | 1.99                     | 0.44              |
| 2:B:272:ARG:NH2    | 2:B:276:ASP:OD2    | 2.50                     | 0.44              |
| 3:C:262:ARG:O      | 8:I:28:PRO:HG2     | 2.17                     | 0.44              |
| 22:C:1031:CLA:H142 | 22:C:1031:CLA:H111 | 1.75                     | 0.44              |
| 25:C:1052:BCR:C33  | 25:C:1052:BCR:C8   | 2.91                     | 0.44              |
| 4:D:161:PRO:CG     | 4:D:170:ALA:CB     | 2.96                     | 0.44              |
| 4:D:170:ALA:C      | 4:D:171:PRO:O      | 2.59                     | 0.44              |
| 4:D:250:ASN:O      | 4:D:252:PHE:N      | 2.51                     | 0.44              |
| 4:D:347:PRO:C      | 4:D:348:ARG:HG3    | 2.43                     | 0.44              |
| 6:F:41:GLN:HG3     | 9:J:27:LEU:CD2     | 2.48                     | 0.44              |
| 10:K:38:VAL:CG1    | 18:Y:36:ILE:HG12   | 2.48                     | 0.44              |
| 13:O:173:ASN:HD22  | 13:O:173:ASN:HA    | 1.54                     | 0.44              |
| 15:U:41:LEU:HD11   | 15:U:74:ILE:HG22   | 2.00                     | 0.44              |
| 1:a:5180:PHE:HD1   | 4:d:5192:THR:HB    | 1.73                     | 0.44              |
| 1:a:5252:HIS:HE2   | 1:a:5264:SER:HB3   | 1.83                     | 0.44              |
| 1:a:5276:ALA:O     | 1:a:5280:VAL:HG23  | 2.17                     | 0.44              |
| 22:a:6007:CLA:HAC1 | 25:a:6044:BCR:C16  | 2.48                     | 0.44              |
| 2:b:5006:TYR:O     | 22:b:6019:CLA:CBA  | 2.66                     | 0.44              |
| 2:b:5134:ASP:H     | 7:h:5015:ASN:ND2   | 2.15                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5237:VAL:HB    | 22:b:6020:CLA:CMD  | 2.48                     | 0.44              |
| 2:b:5323:GLY:C     | 4:d:5293:LEU:HD23  | 2.43                     | 0.44              |
| 3:c:5064:ALA:O     | 3:c:5068:THR:HB    | 2.18                     | 0.44              |
| 3:c:5118:HIS:O     | 3:c:5119:LEU:C     | 2.61                     | 0.44              |
| 3:c:5139:THR:HG23  | 3:c:5142:GLU:CG    | 2.48                     | 0.44              |
| 3:c:5166:ILE:CD1   | 3:c:5248:GLY:HA3   | 2.45                     | 0.44              |
| 3:c:5204:LEU:O     | 3:c:5205:ASP:C     | 2.61                     | 0.44              |
| 3:c:5262:ARG:O     | 8:i:5028:PRO:HG2   | 2.17                     | 0.44              |
| 3:c:5327:ASN:ND2   | 3:c:5330:SER:C     | 2.75                     | 0.44              |
| 22:c:6026:CLA:H142 | 22:c:6026:CLA:H111 | 1.69                     | 0.44              |
| 4:d:5031:GLY:O     | 4:d:5032:TRP:C     | 2.61                     | 0.44              |
| 4:d:5046:GLY:CA    | 25:d:6050:BCR:H10C | 2.48                     | 0.44              |
| 4:d:5096:GLU:HG2   | 4:d:5097:ALA:H     | 1.82                     | 0.44              |
| 4:d:5250:ASN:O     | 4:d:5252:PHE:N     | 2.51                     | 0.44              |
| 7:h:5012:ARG:N     | 7:h:5013:PRO:CD    | 2.79                     | 0.44              |
| 22:h:6017:CLA:H3A  | 22:h:6017:CLA:CGA  | 2.46                     | 0.44              |
| 10:k:5012:PRO:HB3  | 20:z:5062:VAL:HG21 | 2.00                     | 0.44              |
| 15:u:5036:ILE:HG22 | 15:u:5042:TYR:CB   | 2.48                     | 0.44              |
| 1:A:95:PRO:HD2     | 1:A:98:GLU:HB2     | 2.00                     | 0.44              |
| 1:A:133:LEU:HB3    | 4:D:252:PHE:HE2    | 1.83                     | 0.44              |
| 1:A:197:PHE:O      | 1:A:198:HIS:C      | 2.61                     | 0.44              |
| 1:A:223:LEU:CD1    | 4:D:265:ARG:HG2    | 2.46                     | 0.44              |
| 2:B:47:PRO:O       | 2:B:48:SER:C       | 2.61                     | 0.44              |
| 2:B:68:ARG:CD      | 22:B:1011:CLA:HED1 | 2.48                     | 0.44              |
| 2:B:101:ILE:O      | 25:B:1047:BCR:H391 | 2.17                     | 0.44              |
| 2:B:167:TRP:C      | 2:B:168:VAL:HG23   | 2.43                     | 0.44              |
| 2:B:407:ASN:O      | 2:B:409:GLN:N      | 2.51                     | 0.44              |
| 2:B:452:THR:HB     | 4:D:291:LEU:CD1    | 2.48                     | 0.44              |
| 2:B:482:ILE:O      | 2:B:483:ASP:CB     | 2.62                     | 0.44              |
| 3:C:305:THR:O      | 3:C:308:GLU:N      | 2.50                     | 0.44              |
| 3:C:448:ALA:C      | 3:C:450:ALA:N      | 2.74                     | 0.44              |
| 29:C:1056:DGD:C2B  | 29:C:1056:DGD:HG12 | 2.40                     | 0.44              |
| 4:D:90:LEU:CD2     | 4:D:109:GLY:H      | 2.31                     | 0.44              |
| 4:D:180:ARG:NH1    | 4:D:184:PHE:CD1    | 2.85                     | 0.44              |
| 4:D:221:THR:CG2    | 4:D:248:THR:HB     | 2.46                     | 0.44              |
| 4:D:303:ILE:HG21   | 12:M:2:GLU:HB3     | 2.00                     | 0.44              |
| 7:H:30:LEU:C       | 22:H:1017:CLA:HMD1 | 2.43                     | 0.44              |
| 10:K:30:VAL:O      | 10:K:32:PHE:N      | 2.50                     | 0.44              |
| 12:M:20:VAL:CG2    | 12:m:5020:VAL:HG11 | 2.48                     | 0.44              |
| 12:M:27:VAL:O      | 12:M:27:VAL:HG12   | 2.18                     | 0.44              |
| 16:V:35:THR:HG23   | 16:V:46:THR:CA     | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:V:106:THR:HA    | 16:V:114:ILE:HG22  | 2.00                     | 0.44              |
| 16:V:126:ILE:O     | 16:V:128:PRO:HD3   | 2.18                     | 0.44              |
| 1:a:5132:GLU:O     | 1:a:5136:ARG:HG2   | 2.17                     | 0.44              |
| 1:a:5143:ILE:CG2   | 1:a:5144:CYS:N     | 2.81                     | 0.44              |
| 1:a:5177:SER:HA    | 1:a:5180:PHE:HD2   | 1.83                     | 0.44              |
| 1:a:5215:HIS:ND1   | 24:a:6043:PQ9:O1   | 2.51                     | 0.44              |
| 1:a:5279:ARG:CZ    | 1:a:5283:VAL:CG2   | 2.95                     | 0.44              |
| 25:a:6044:BCR:C37  | 25:a:6044:BCR:C30  | 2.62                     | 0.44              |
| 2:b:5136:PRO:HB3   | 2:b:5221:PRO:HG3   | 2.00                     | 0.44              |
| 2:b:5291:SER:O     | 2:b:5296:ALA:HB3   | 2.18                     | 0.44              |
| 3:c:5075:PHE:O     | 10:k:5010:LYS:HE3  | 2.18                     | 0.44              |
| 3:c:5223:TRP:HD1   | 3:c:5224:ILE:HD13  | 1.83                     | 0.44              |
| 3:c:5305:THR:O     | 3:c:5308:GLU:N     | 2.50                     | 0.44              |
| 3:c:5385:GLN:HB3   | 3:c:5386:PRO:CD    | 2.48                     | 0.44              |
| 22:c:6025:CLA:CHB  | 22:c:6025:CLA:O2A  | 2.60                     | 0.44              |
| 4:d:5217:THR:HG23  | 4:d:5218:VAL:N     | 2.32                     | 0.44              |
| 4:d:5253:TRP:HD1   | 24:d:6042:PQ9:H92  | 1.82                     | 0.44              |
| 4:d:5303:ILE:HG21  | 12:m:5002:GLU:HB3  | 2.00                     | 0.44              |
| 4:d:5326:ARG:HG3   | 4:d:5326:ARG:NH1   | 2.32                     | 0.44              |
| 24:d:6042:PQ9:H393 | 11:l:5026:VAL:CG1  | 2.48                     | 0.44              |
| 6:f:5041:GLN:HG3   | 9:j:5027:LEU:CD2   | 2.48                     | 0.44              |
| 9:j:5007:ARG:HG2   | 9:j:5007:ARG:NH1   | 2.31                     | 0.44              |
| 10:k:5017:ILE:HB   | 10:k:5018:PHE:CD1  | 2.53                     | 0.44              |
| 12:m:5033:GLN:C    | 12:m:5035:SER:H    | 2.26                     | 0.44              |
| 1:A:213:ALA:CB     | 23:D:1039:PHO:HBC1 | 2.47                     | 0.43              |
| 1:A:341:LEU:O      | 1:A:343:LEU:N      | 2.48                     | 0.43              |
| 2:B:124:ARG:HA     | 2:B:124:ARG:HD3    | 1.74                     | 0.43              |
| 2:B:153:PHE:O      | 2:B:154:GLY:C      | 2.59                     | 0.43              |
| 22:B:1023:CLA:H91  | 22:B:1024:CLA:H152 | 1.88                     | 0.43              |
| 22:B:1023:CLA:H61  | 22:B:1023:CLA:H2   | 1.47                     | 0.43              |
| 3:C:86:LEU:HB3     | 3:C:90:PRO:HD3     | 1.98                     | 0.43              |
| 3:C:87:ILE:HG13    | 3:C:88:LEU:N       | 2.32                     | 0.43              |
| 3:C:266:TRP:HB3    | 3:C:271:TYR:HH     | 1.79                     | 0.43              |
| 3:C:281:MET:CG     | 3:C:285:ILE:HD11   | 2.48                     | 0.43              |
| 3:C:379:LYS:O      | 3:C:380:ILE:C      | 2.61                     | 0.43              |
| 22:C:1026:CLA:HBB2 | 22:K:1034:CLA:H11  | 1.98                     | 0.43              |
| 22:C:1028:CLA:C1C  | 29:C:1056:DGD:HA31 | 2.47                     | 0.43              |
| 22:C:1029:CLA:H11  | 22:C:1029:CLA:C1A  | 2.47                     | 0.43              |
| 4:D:270:PHE:O      | 4:D:270:PHE:CD1    | 2.70                     | 0.43              |
| 28:D:1062:MGE:O1A  | 28:D:1062:MGE:C4B  | 2.66                     | 0.43              |
| 5:E:10:PHE:CE1     | 6:F:19:ARG:HD2     | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:K:28:ILE:HA     | 10:K:31:LEU:HG     | 1.99                     | 0.43              |
| 11:L:24:ILE:CD1    | 12:M:18:PRO:HB2    | 2.48                     | 0.43              |
| 13:O:44:LYS:HB3    | 13:O:72:GLN:OE1    | 2.18                     | 0.43              |
| 16:V:90:PRO:HD2    | 16:V:92:ARG:NH2    | 2.33                     | 0.43              |
| 1:a:5058:VAL:CG2   | 1:a:5083:VAL:HG23  | 2.48                     | 0.43              |
| 1:a:5129:ARG:NH1   | 4:d:5256:ILE:HD12  | 2.32                     | 0.43              |
| 1:a:5145:VAL:O     | 1:a:5146:ALA:C     | 2.59                     | 0.43              |
| 2:b:5167:TRP:C     | 2:b:5168:VAL:HG23  | 2.43                     | 0.43              |
| 2:b:5272:ARG:HA    | 2:b:5319:PRO:HD2   | 2.00                     | 0.43              |
| 2:b:5407:ASN:O     | 2:b:5409:GLN:N     | 2.51                     | 0.43              |
| 3:c:5127:PHE:C     | 3:c:5130:VAL:HG12  | 2.42                     | 0.43              |
| 3:c:5176:VAL:O     | 3:c:5180:MET:N     | 2.45                     | 0.43              |
| 3:c:5210:PHE:HE1   | 3:c:5239:TRP:CE3   | 2.35                     | 0.43              |
| 3:c:5420:VAL:HG21  | 3:c:5425:TRP:HZ2   | 1.83                     | 0.43              |
| 3:c:5429:SER:O     | 3:c:5432:VAL:CG1   | 2.60                     | 0.43              |
| 3:c:5457:LYS:HD2   | 4:d:5224:GLN:NE2   | 2.33                     | 0.43              |
| 22:c:6028:CLA:H62  | 29:c:6057:DGD:HA42 | 2.00                     | 0.43              |
| 22:d:6005:CLA:H203 | 22:d:6005:CLA:H161 | 1.75                     | 0.43              |
| 7:h:5056:ASP:C     | 7:h:5058:VAL:H     | 2.26                     | 0.43              |
| 13:o:5064:TYR:HA   | 13:o:5271:PRO:HA   | 1.99                     | 0.43              |
| 13:o:5163:THR:C    | 13:o:5165:SER:H    | 2.26                     | 0.43              |
| 20:z:5026:ALA:CB   | 20:z:5040:ILE:HD11 | 2.47                     | 0.43              |
| 1:A:177:SER:HA     | 1:A:180:PHE:HD2    | 1.83                     | 0.43              |
| 23:A:1038:PHO:OBD  | 23:A:1038:PHO:CED  | 2.66                     | 0.43              |
| 2:B:28:ALA:HB2     | 2:B:107:LEU:CB     | 2.48                     | 0.43              |
| 2:B:63:LEU:N       | 2:B:64:PRO:HD3     | 2.33                     | 0.43              |
| 3:C:45:LEU:HB3     | 3:C:46:SER:H       | 1.59                     | 0.43              |
| 3:C:69:LEU:HD21    | 3:C:116:VAL:HG22   | 2.01                     | 0.43              |
| 3:C:118:HIS:O      | 3:C:119:LEU:C      | 2.61                     | 0.43              |
| 3:C:204:LEU:O      | 3:C:205:ASP:C      | 2.61                     | 0.43              |
| 3:C:284:PHE:HB3    | 29:C:1055:DGD:HB81 | 2.00                     | 0.43              |
| 3:C:293:ASN:OD1    | 3:C:294:ASN:N      | 2.51                     | 0.43              |
| 3:C:405:ASN:OD1    | 3:C:405:ASN:C      | 2.61                     | 0.43              |
| 3:C:460:ASP:OD1    | 3:C:462:GLU:HG2    | 2.18                     | 0.43              |
| 22:C:1026:CLA:HBB1 | 22:K:1034:CLA:HMD2 | 2.00                     | 0.43              |
| 22:C:1032:CLA:HBD  | 22:C:1032:CLA:HAA1 | 2.01                     | 0.43              |
| 22:C:1035:CLA:HMC3 | 22:K:1034:CLA:CMB  | 2.48                     | 0.43              |
| 29:C:1057:DGD:O2D  | 9:J:32:ALA:HB1     | 2.18                     | 0.43              |
| 4:D:267:LEU:C      | 4:D:267:LEU:CD2    | 2.91                     | 0.43              |
| 22:D:1005:CLA:HBC1 | 22:D:1004:CLA:CBB  | 2.34                     | 0.43              |
| 5:E:8:ARG:HB2      | 6:F:13:TYR:CB      | 2.48                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:O:70:CYS:HB2    | 13:O:105:ASP:CB    | 2.47                     | 0.43              |
| 2:b:5049:ASP:C     | 2:b:5051:VAL:H     | 2.26                     | 0.43              |
| 2:b:5226:TYR:O     | 2:b:5226:TYR:CD2   | 2.66                     | 0.43              |
| 2:b:5249:ALA:CB    | 2:b:5459:ALA:CB    | 2.95                     | 0.43              |
| 2:b:5345:VAL:HG23  | 2:b:5345:VAL:O     | 2.18                     | 0.43              |
| 22:b:6011:CLA:CGD  | 22:b:6013:CLA:H11  | 2.42                     | 0.43              |
| 22:b:6019:CLA:H122 | 22:b:6019:CLA:H162 | 1.51                     | 0.43              |
| 22:b:6022:CLA:H152 | 12:m:5024:ILE:HG21 | 1.99                     | 0.43              |
| 3:c:5056:HIS:O     | 3:c:5059:LEU:N     | 2.52                     | 0.43              |
| 3:c:5087:ILE:HG13  | 3:c:5088:LEU:N     | 2.33                     | 0.43              |
| 3:c:5293:ASN:OD1   | 3:c:5294:ASN:N     | 2.51                     | 0.43              |
| 3:c:5330:SER:HB2   | 13:o:5126:GLY:O    | 2.17                     | 0.43              |
| 22:c:6036:CLA:H13  | 22:c:6036:CLA:H102 | 1.50                     | 0.43              |
| 24:d:6042:PQ9:H42  | 24:d:6042:PQ9:H391 | 0.62                     | 0.43              |
| 7:h:5030:LEU:C     | 22:h:6017:CLA:HMD1 | 2.43                     | 0.43              |
| 13:o:5041:LEU:C    | 13:o:5043:ASN:N    | 2.77                     | 0.43              |
| 25:t:1046:BCR:C33  | 25:t:1046:BCR:C8   | 2.72                     | 0.43              |
| 15:u:5070:ARG:CZ   | 15:u:5074:ILE:HD11 | 2.49                     | 0.43              |
| 1:A:51:ALA:O       | 1:A:55:ALA:HB3     | 2.18                     | 0.43              |
| 1:A:285:PHE:O      | 1:A:288:LEU:HB2    | 2.19                     | 0.43              |
| 22:A:1007:CLA:HAC1 | 25:A:1044:BCR:C16  | 2.48                     | 0.43              |
| 22:A:1007:CLA:C14  | 8:I:13:THR:OG1     | 2.66                     | 0.43              |
| 2:B:46:ASP:CG      | 2:B:48:SER:OG      | 2.61                     | 0.43              |
| 2:B:69:LEU:HD12    | 2:B:69:LEU:HA      | 1.84                     | 0.43              |
| 22:B:1015:CLA:H71  | 22:B:1015:CLA:H42  | 1.94                     | 0.43              |
| 22:B:1023:CLA:H151 | 22:B:1024:CLA:C4A  | 2.48                     | 0.43              |
| 25:B:1047:BCR:H272 | 25:t:1046:BCR:H341 | 2.00                     | 0.43              |
| 3:C:56:HIS:O       | 3:C:59:LEU:N       | 2.52                     | 0.43              |
| 3:C:75:PHE:O       | 10:K:10:LYS:HE3    | 2.18                     | 0.43              |
| 3:C:265:ILE:HG23   | 3:C:270:ALA:CB     | 2.48                     | 0.43              |
| 3:C:337:LEU:HD22   | 3:C:342:MET:HG3    | 1.99                     | 0.43              |
| 3:C:440:GLY:O      | 3:C:442:LEU:N      | 2.50                     | 0.43              |
| 22:C:1035:CLA:H152 | 20:Z:20:VAL:HG13   | 1.98                     | 0.43              |
| 4:D:48:TRP:CD1     | 23:D:1039:PHO:H162 | 2.53                     | 0.43              |
| 4:D:57:SER:OG      | 4:D:65:SER:CB      | 2.64                     | 0.43              |
| 4:D:96:GLU:HG2     | 4:D:97:ALA:H       | 1.82                     | 0.43              |
| 24:D:1042:PQ9:H393 | 11:L:26:VAL:CG1    | 2.48                     | 0.43              |
| 22:H:1017:CLA:H93  | 22:H:1017:CLA:H62  | 1.59                     | 0.43              |
| 9:J:10:LEU:CD2     | 9:J:11:TRP:H       | 2.31                     | 0.43              |
| 13:O:184:ASP:OD2   | 13:O:188:ARG:NH1   | 2.50                     | 0.43              |
| 15:U:36:ILE:HG22   | 15:U:42:TYR:CB     | 2.48                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:U:36:ILE:HA     | 15:U:42:TYR:HB2    | 2.01                     | 0.43              |
| 16:V:95:ILE:O      | 16:V:99:VAL:HG23   | 2.18                     | 0.43              |
| 1:a:5037:MET:SD    | 1:a:5126:TYR:HA    | 2.59                     | 0.43              |
| 1:a:5038:ILE:O     | 1:a:5042:LEU:HD23  | 2.18                     | 0.43              |
| 1:a:5133:LEU:HD23  | 4:d:5252:PHE:CD2   | 2.53                     | 0.43              |
| 23:a:6038:PHO:O1D  | 23:a:6038:PHO:C2A  | 2.57                     | 0.43              |
| 2:b:5113:TRP:HD1   | 2:b:5114:HIS:N     | 2.16                     | 0.43              |
| 2:b:5185:TRP:HZ3   | 2:b:5204:ALA:HB2   | 1.83                     | 0.43              |
| 2:b:5278:SER:O     | 2:b:5279:TYR:C     | 2.61                     | 0.43              |
| 2:b:5298:LEU:HD11  | 2:b:5302:TRP:NE1   | 2.27                     | 0.43              |
| 22:b:6010:CLA:C2D  | 22:b:6011:CLA:HMB1 | 2.48                     | 0.43              |
| 22:b:6022:CLA:C14  | 22:b:6022:CLA:C7   | 2.70                     | 0.43              |
| 22:b:6022:CLA:H62  | 22:b:6022:CLA:H141 | 1.75                     | 0.43              |
| 3:c:5029:GLU:C     | 3:c:5029:GLU:CD    | 2.86                     | 0.43              |
| 3:c:5082:TYR:HD1   | 3:c:5419:PHE:HE2   | 1.67                     | 0.43              |
| 3:c:5143:TYR:CE2   | 22:c:6037:CLA:HED2 | 2.53                     | 0.43              |
| 3:c:5265:ILE:HG23  | 3:c:5270:ALA:CB    | 2.48                     | 0.43              |
| 3:c:5320:ARG:O     | 3:c:5324:LEU:HB2   | 2.17                     | 0.43              |
| 3:c:5321:ASP:HB2   | 3:c:5340:TYR:HE1   | 1.83                     | 0.43              |
| 3:c:5348:GLU:OE2   | 3:c:5373:ASN:HB3   | 2.18                     | 0.43              |
| 4:d:5185:PHE:O     | 4:d:5190:ASN:N     | 2.50                     | 0.43              |
| 22:d:6005:CLA:H41  | 22:d:6005:CLA:H61  | 1.58                     | 0.43              |
| 6:f:5015:ILE:HD12  | 31:f:6040:HEM:CMD  | 2.49                     | 0.43              |
| 10:k:5018:PHE:CD1  | 10:k:5018:PHE:N    | 2.86                     | 0.43              |
| 10:k:5027:VAL:O    | 10:k:5031:LEU:HG   | 2.18                     | 0.43              |
| 25:k:6052:BCR:C33  | 25:k:6052:BCR:C8   | 2.91                     | 0.43              |
| 12:m:5009:ILE:CG2  | 12:m:5013:LEU:HD23 | 2.48                     | 0.43              |
| 13:o:5074:THR:HG22 | 13:o:5263:GLY:HA2  | 2.00                     | 0.43              |
| 15:u:5025:ILE:HG21 | 15:u:5035:PHE:CE2  | 2.47                     | 0.43              |
| 16:v:5035:THR:HG23 | 16:v:5046:THR:CA   | 2.47                     | 0.43              |
| 17:x:5013:THR:HG22 | 17:x:5014:PRO:HD2  | 2.00                     | 0.43              |
| 1:A:93:PHE:HB2     | 3:C:218:PHE:CD2    | 2.47                     | 0.43              |
| 1:A:161:TYR:CZ     | 1:A:186:PHE:CE2    | 3.06                     | 0.43              |
| 23:A:1038:PHO:HBA1 | 23:A:1038:PHO:H3A  | 1.26                     | 0.43              |
| 2:B:61:PHE:HB2     | 22:B:1015:CLA:CMA  | 2.48                     | 0.43              |
| 2:B:103:LEU:HD12   | 2:B:103:LEU:C      | 2.44                     | 0.43              |
| 2:B:113:TRP:HD1    | 2:B:114:HIS:N      | 2.16                     | 0.43              |
| 2:B:185:TRP:HZ3    | 2:B:204:ALA:HB2    | 1.84                     | 0.43              |
| 2:B:226:TYR:O      | 2:B:226:TYR:CD2    | 2.66                     | 0.43              |
| 2:B:307:GLU:O      | 2:B:308:LYS:C      | 2.61                     | 0.43              |
| 22:B:1013:CLA:H111 | 22:B:1013:CLA:H142 | 1.73                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1022:CLA:CBC  | 22:B:1022:CLA:CHD  | 2.79                     | 0.43              |
| 22:B:1023:CLA:CMB  | 22:B:1023:CLA:HBB1 | 2.48                     | 0.43              |
| 22:B:1024:CLA:H111 | 22:B:1024:CLA:H143 | 1.77                     | 0.43              |
| 3:C:64:ALA:O       | 3:C:68:THR:HB      | 2.18                     | 0.43              |
| 3:C:123:ALA:HA     | 25:C:1052:BCR:C14  | 2.48                     | 0.43              |
| 3:C:321:ASP:HB2    | 3:C:340:TYR:HE1    | 1.83                     | 0.43              |
| 22:C:1026:CLA:C3   | 22:C:1026:CLA:CGA  | 2.96                     | 0.43              |
| 22:C:1031:CLA:CMD  | 22:C:1033:CLA:H162 | 2.48                     | 0.43              |
| 4:D:53:THR:HG23    | 4:D:67:TYR:HE2     | 1.83                     | 0.43              |
| 4:D:90:LEU:O       | 22:D:1008:CLA:HED1 | 2.18                     | 0.43              |
| 10:K:27:VAL:O      | 10:K:31:LEU:HG     | 2.18                     | 0.43              |
| 25:K:1051:BCR:C23  | 25:K:1051:BCR:H392 | 2.48                     | 0.43              |
| 16:V:47:LEU:HD21   | 16:V:51:GLN:HB2    | 2.01                     | 0.43              |
| 18:Y:28:ILE:CG1    | 18:Y:29:GLY:N      | 2.78                     | 0.43              |
| 1:a:5091:LEU:HD23  | 1:a:5091:LEU:HA    | 1.88                     | 0.43              |
| 1:a:5213:ALA:CB    | 23:d:6039:PHO:HBC1 | 2.48                     | 0.43              |
| 1:a:5301:ASN:HB3   | 3:c:5407:VAL:HG11  | 2.00                     | 0.43              |
| 1:a:5309:ALA:O     | 1:a:5311:GLY:N     | 2.51                     | 0.43              |
| 22:a:6007:CLA:C14  | 8:i:5013:THR:OG1   | 2.66                     | 0.43              |
| 23:a:6038:PHO:C9   | 22:d:6005:CLA:C17  | 2.97                     | 0.43              |
| 2:b:5028:ALA:HB2   | 2:b:5107:LEU:CB    | 2.48                     | 0.43              |
| 2:b:5247:PHE:CE1   | 2:b:5251:VAL:CG2   | 3.01                     | 0.43              |
| 2:b:5331:ASN:C     | 2:b:5333:GLY:N     | 2.76                     | 0.43              |
| 22:b:6021:CLA:H62  | 28:b:6060:MGE:H231 | 2.01                     | 0.43              |
| 3:c:5087:ILE:HG13  | 3:c:5088:LEU:H     | 1.83                     | 0.43              |
| 3:c:5117:VAL:HG21  | 22:c:6027:CLA:C4   | 2.49                     | 0.43              |
| 22:c:6026:CLA:HBB1 | 22:k:6034:CLA:HMD2 | 2.01                     | 0.43              |
| 22:c:6032:CLA:HAA1 | 22:c:6032:CLA:HBD  | 2.01                     | 0.43              |
| 22:c:6033:CLA:H202 | 22:c:6033:CLA:H162 | 1.78                     | 0.43              |
| 29:c:6057:DGD:HB72 | 28:d:6059:MGE:H7B1 | 1.99                     | 0.43              |
| 4:d:5027:PHE:CD1   | 6:f:5019:ARG:HG3   | 2.52                     | 0.43              |
| 4:d:5111:TRP:O     | 4:d:5112:THR:C     | 2.61                     | 0.43              |
| 4:d:5195:PRO:O     | 4:d:5196:PHE:C     | 2.61                     | 0.43              |
| 4:d:5247:VAL:C     | 4:d:5249:ALA:H     | 2.26                     | 0.43              |
| 5:e:5008:ARG:HB2   | 6:f:5013:TYR:CB    | 2.48                     | 0.43              |
| 11:l:5026:VAL:CG1  | 11:l:5027:LEU:N    | 2.80                     | 0.43              |
| 13:o:5044:LYS:HB3  | 13:o:5072:GLN:OE1  | 2.18                     | 0.43              |
| 16:v:5095:ILE:O    | 16:v:5099:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:13:LEU:H       | 1:A:13:LEU:CD1     | 2.27                     | 0.43              |
| 2:B:33:TRP:HA      | 2:B:36:SER:HB2     | 1.99                     | 0.43              |
| 2:B:297:THR:O      | 2:B:298:LEU:C      | 2.60                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:359:MET:HB3    | 2:B:425:ILE:HG23   | 2.00                     | 0.43              |
| 2:B:460:LEU:O      | 4:D:280:TRP:CZ3    | 2.70                     | 0.43              |
| 22:B:1021:CLA:H62  | 28:B:1060:MGE:H231 | 2.01                     | 0.43              |
| 3:C:29:GLU:C       | 3:C:29:GLU:CD      | 2.86                     | 0.43              |
| 3:C:81:MET:SD      | 3:C:90:PRO:HA      | 2.57                     | 0.43              |
| 3:C:224:ILE:CG2    | 25:C:1054:BCR:H381 | 2.34                     | 0.43              |
| 4:D:16:ASP:O       | 4:D:20:ASP:HB2     | 2.18                     | 0.43              |
| 4:D:31:GLY:O       | 4:D:32:TRP:C       | 2.61                     | 0.43              |
| 4:D:103:ARG:HA     | 4:D:106:GLN:HE21   | 1.83                     | 0.43              |
| 4:D:337:GLU:HG2    | 4:D:339:PHE:CZ     | 2.53                     | 0.43              |
| 10:K:35:LEU:O      | 10:K:36:ALA:C      | 2.61                     | 0.43              |
| 12:M:9:ILE:CG2     | 12:M:13:LEU:HD23   | 2.48                     | 0.43              |
| 13:O:245:GLN:C     | 13:O:246:LEU:HD23  | 2.43                     | 0.43              |
| 15:U:70:ARG:CZ     | 15:U:74:ILE:HD11   | 2.49                     | 0.43              |
| 16:V:45:ILE:HG22   | 16:V:45:ILE:O      | 2.19                     | 0.43              |
| 16:V:101:TYR:HE1   | 16:V:118:HIS:ND1   | 2.14                     | 0.43              |
| 17:X:37:LEU:HD23   | 17:X:37:LEU:HA     | 1.74                     | 0.43              |
| 1:a:5204:GLY:O     | 1:a:5208:GLY:N     | 2.47                     | 0.43              |
| 1:a:5286:ALA:O     | 1:a:5289:GLY:N     | 2.51                     | 0.43              |
| 1:a:5290:ILE:HG12  | 22:a:6003:CLA:OBD  | 2.19                     | 0.43              |
| 2:b:5006:TYR:CD2   | 2:b:5006:TYR:N     | 2.76                     | 0.43              |
| 2:b:5006:TYR:CE1   | 28:b:6060:MGE:H2D  | 2.53                     | 0.43              |
| 2:b:5035:GLY:O     | 2:b:5039:LEU:HG    | 2.18                     | 0.43              |
| 2:b:5046:ASP:CG    | 2:b:5048:SER:OG    | 2.61                     | 0.43              |
| 2:b:5359:MET:HB3   | 2:b:5425:ILE:HG23  | 2.00                     | 0.43              |
| 2:b:5424:ALA:C     | 2:b:5426:PHE:N     | 2.77                     | 0.43              |
| 4:d:5096:GLU:H     | 4:d:5096:GLU:CD    | 2.26                     | 0.43              |
| 4:d:5331:PRO:HD3   | 4:d:5341:PHE:HE2   | 1.82                     | 0.43              |
| 22:d:6004:CLA:HAA2 | 22:d:6004:CLA:CBD  | 2.49                     | 0.43              |
| 11:l:5024:ILE:C    | 11:l:5026:VAL:N    | 2.76                     | 0.43              |
| 13:o:5092:VAL:HG12 | 13:o:5093:PRO:N    | 2.33                     | 0.43              |
| 14:t:5028:ARG:HA   | 14:t:5028:ARG:HE   | 1.83                     | 0.43              |
| 15:u:5051:LYS:O    | 15:u:5052:ASN:O    | 2.36                     | 0.43              |
| 18:y:5043:ARG:CZ   | 20:z:5029:SER:HB3  | 2.49                     | 0.43              |
| 1:A:59:ASP:OD2     | 1:A:59:ASP:N       | 2.51                     | 0.43              |
| 1:A:143:ILE:CG2    | 1:A:144:CYS:N      | 2.81                     | 0.43              |
| 1:A:218:LEU:O      | 1:A:219:VAL:C      | 2.59                     | 0.43              |
| 1:A:271:LEU:O      | 1:A:274:PHE:N      | 2.52                     | 0.43              |
| 1:A:281:VAL:CG1    | 1:A:285:PHE:HE1    | 2.32                     | 0.43              |
| 1:A:320:ILE:O      | 1:A:323:ARG:N      | 2.50                     | 0.43              |
| 1:A:323:ARG:HD2    | 1:A:323:ARG:HA     | 1.72                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:A:1038:PHO:C9  | 22:D:1005:CLA:C17  | 2.97                     | 0.43              |
| 23:A:1038:PHO:C4  | 23:A:1038:PHO:C7   | 2.93                     | 0.43              |
| 24:A:1043:PQ9:C45 | 24:A:1043:PQ9:C40  | 2.96                     | 0.43              |
| 2:B:6:TYR:CE1     | 28:B:1060:MGE:H2D  | 2.53                     | 0.43              |
| 2:B:12:LEU:HD23   | 2:B:19:LEU:HA      | 1.99                     | 0.43              |
| 2:B:15:ASP:CG     | 2:B:18:ARG:HG3     | 2.43                     | 0.43              |
| 2:B:188:ASP:OD1   | 7:H:58:VAL:HA      | 2.19                     | 0.43              |
| 2:B:328:GLY:O     | 2:B:444:ARG:HG2    | 2.18                     | 0.43              |
| 2:B:345:VAL:HG23  | 2:B:345:VAL:O      | 2.18                     | 0.43              |
| 2:B:347:ARG:HG2   | 2:B:347:ARG:HH11   | 1.83                     | 0.43              |
| 2:B:468:TRP:CE2   | 22:B:1019:CLA:HED2 | 2.53                     | 0.43              |
| 3:C:81:MET:SD     | 3:C:89:ILE:HG22    | 2.59                     | 0.43              |
| 3:C:139:THR:HG23  | 3:C:139:THR:O      | 2.18                     | 0.43              |
| 3:C:142:GLU:CD    | 3:C:143:TYR:N      | 2.76                     | 0.43              |
| 3:C:229:ASN:ND2   | 3:C:232:ASP:OD2    | 2.47                     | 0.43              |
| 3:C:438:LEU:HD13  | 3:C:442:LEU:CD1    | 2.49                     | 0.43              |
| 22:C:1027:CLA:HHC | 22:C:1027:CLA:CBB  | 2.48                     | 0.43              |
| 4:D:46:GLY:CA     | 25:D:1050:BCR:H10C | 2.48                     | 0.43              |
| 4:D:67:TYR:O      | 4:D:70:GLY:N       | 2.47                     | 0.43              |
| 4:D:158:LEU:O     | 4:D:162:LEU:CG     | 2.66                     | 0.43              |
| 25:D:1050:BCR:C19 | 28:D:1059:MGE:H102 | 2.48                     | 0.43              |
| 7:H:56:ASP:C      | 7:H:58:VAL:H       | 2.26                     | 0.43              |
| 13:O:58:ILE:HG23  | 13:O:160:THR:O     | 2.18                     | 0.43              |
| 13:O:209:ALA:O    | 13:O:210:ARG:C     | 2.62                     | 0.43              |
| 15:U:55:TYR:N     | 15:U:55:TYR:CD1    | 2.82                     | 0.43              |
| 20:Z:4:LEU:HD12   | 20:Z:4:LEU:O       | 2.17                     | 0.43              |
| 20:Z:44:SER:O     | 20:Z:48:ILE:CD1    | 2.66                     | 0.43              |
| 1:a:5027:ARG:HG3  | 1:a:5027:ARG:HH11  | 1.84                     | 0.43              |
| 1:a:5039:PRO:CD   | 22:a:6007:CLA:HBB2 | 2.45                     | 0.43              |
| 1:a:5271:LEU:O    | 1:a:5274:PHE:N     | 2.52                     | 0.43              |
| 1:a:5281:VAL:CG1  | 1:a:5285:PHE:HE1   | 2.32                     | 0.43              |
| 1:a:5289:GLY:O    | 1:a:5293:MET:HE3   | 2.18                     | 0.43              |
| 1:a:5310:LYS:HD3  | 1:a:5312:ASN:ND2   | 2.33                     | 0.43              |
| 1:a:5330:VAL:HG11 | 4:d:5347:PRO:O     | 2.19                     | 0.43              |
| 2:b:5068:ARG:CD   | 22:b:6011:CLA:HED1 | 2.48                     | 0.43              |
| 2:b:5313:ASP:OD2  | 2:b:5358:ARG:NH2   | 2.50                     | 0.43              |
| 2:b:5328:GLY:O    | 2:b:5444:ARG:HG2   | 2.18                     | 0.43              |
| 3:c:5058:GLY:O    | 3:c:5059:LEU:C     | 2.61                     | 0.43              |
| 3:c:5069:LEU:HD21 | 3:c:5116:VAL:HG22  | 2.00                     | 0.43              |
| 3:c:5089:ILE:N    | 3:c:5090:PRO:CD    | 2.80                     | 0.43              |
| 3:c:5117:VAL:CG2  | 22:c:6027:CLA:H162 | 2.49                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5142:GLU:CD    | 3:c:5143:TYR:N     | 2.76                     | 0.43              |
| 3:c:5281:MET:CG    | 3:c:5285:ILE:HD11  | 2.48                     | 0.43              |
| 3:c:5322:GLN:NE2   | 3:c:5381:LYS:HG2   | 2.34                     | 0.43              |
| 3:c:5460:ASP:OD1   | 3:c:5462:GLU:HG2   | 2.18                     | 0.43              |
| 4:d:5014:TRP:O     | 4:d:5017:ILE:CG1   | 2.67                     | 0.43              |
| 4:d:5160:TYR:CZ    | 27:d:6068:IOD:I    | 3.40                     | 0.43              |
| 7:h:5041:PHE:CD1   | 25:h:6049:BCR:H362 | 2.49                     | 0.43              |
| 13:o:5260:LYS:O    | 13:o:5261:ILE:HD13 | 2.19                     | 0.43              |
| 16:v:5081:ARG:O    | 16:v:5082:THR:C    | 2.62                     | 0.43              |
| 16:v:5105:PRO:HD3  | 16:v:5120:SER:HB3  | 2.01                     | 0.43              |
| 1:A:60:ILE:O       | 1:A:61:ASP:O       | 2.37                     | 0.43              |
| 1:A:219:VAL:HG11   | 4:D:268:HIS:CD2    | 2.54                     | 0.43              |
| 1:A:259:ILE:HD13   | 24:A:1043:PQ9:C24  | 2.38                     | 0.43              |
| 1:A:259:ILE:N      | 4:D:128:ARG:NH2    | 2.58                     | 0.43              |
| 1:A:301:ASN:HB3    | 3:C:407:VAL:HG11   | 2.00                     | 0.43              |
| 1:A:330:VAL:HG11   | 4:D:347:PRO:O      | 2.19                     | 0.43              |
| 24:A:1043:PQ9:H311 | 24:A:1043:PQ9:H291 | 1.68                     | 0.43              |
| 2:B:6:TYR:OH       | 28:B:1060:MGE:H3D  | 2.19                     | 0.43              |
| 2:B:278:SER:O      | 2:B:279:TYR:C      | 2.61                     | 0.43              |
| 2:B:314:TYR:O      | 2:B:315:ILE:C      | 2.62                     | 0.43              |
| 2:B:389:LYS:HB3    | 2:B:390:TYR:CE1    | 2.54                     | 0.43              |
| 22:B:1011:CLA:H42  | 22:B:1011:CLA:O2A  | 2.19                     | 0.43              |
| 22:B:1021:CLA:CED  | 22:B:1021:CLA:C2   | 2.89                     | 0.43              |
| 28:B:1060:MGE:O1B  | 28:B:1060:MGE:C3G  | 2.63                     | 0.43              |
| 3:C:145:SER:O      | 3:C:147:PHE:N      | 2.52                     | 0.43              |
| 3:C:220:GLY:C      | 3:C:221:GLU:HG3    | 2.44                     | 0.43              |
| 3:C:298:PRO:O      | 3:C:300:GLU:OE1    | 2.36                     | 0.43              |
| 3:C:332:GLN:NE2    | 13:O:175:PRO:HG3   | 2.34                     | 0.43              |
| 3:C:343:ARG:NH1    | 3:C:348:GLU:CB     | 2.82                     | 0.43              |
| 3:C:348:GLU:OE2    | 3:C:373:ASN:HB3    | 2.18                     | 0.43              |
| 4:D:185:PHE:O      | 4:D:190:ASN:N      | 2.50                     | 0.43              |
| 4:D:277:THR:HG22   | 4:D:278:GLY:N      | 2.34                     | 0.43              |
| 5:E:68:ASP:H       | 5:E:75:GLN:HE21    | 1.65                     | 0.43              |
| 6:F:41:GLN:HG3     | 9:J:27:LEU:HG      | 2.01                     | 0.43              |
| 9:J:7:ARG:HG2      | 9:J:7:ARG:NH1      | 2.31                     | 0.43              |
| 22:K:1034:CLA:C4   | 22:K:1034:CLA:HBA1 | 2.49                     | 0.43              |
| 13:O:59:ASP:CG     | 13:O:61:SER:HB2    | 2.43                     | 0.43              |
| 13:O:69:LEU:HD12   | 13:O:69:LEU:C      | 2.44                     | 0.43              |
| 13:O:92:VAL:HG12   | 13:O:93:PRO:N      | 2.33                     | 0.43              |
| 13:O:160:THR:O     | 13:O:160:THR:CG2   | 2.66                     | 0.43              |
| 13:O:172:PHE:CB    | 13:O:221:GLY:HA3   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:O:184:ASP:OD1  | 13:O:188:ARG:HB2   | 2.18                     | 0.43              |
| 14:T:14:ILE:HG21  | 25:T:6046:BCR:H352 | 2.00                     | 0.43              |
| 1:a:5102:LEU:HD12 | 1:a:5102:LEU:C     | 2.44                     | 0.43              |
| 1:a:5142:TRP:HE1  | 4:d:5219:GLU:HB3   | 1.84                     | 0.43              |
| 1:a:5325:ASN:HD22 | 1:a:5325:ASN:HA    | 1.51                     | 0.43              |
| 1:a:5340:PRO:CD   | 15:u:5103:TYR:HE2  | 2.32                     | 0.43              |
| 22:a:6003:CLA:HHD | 22:a:6003:CLA:CBC  | 2.33                     | 0.43              |
| 22:a:6003:CLA:HAB | 22:d:6004:CLA:C4B  | 2.49                     | 0.43              |
| 22:a:6006:CLA:CAA | 29:c:6057:DGD:HBN2 | 2.48                     | 0.43              |
| 2:b:5003:LEU:O    | 11:l:5010:VAL:HA   | 2.19                     | 0.43              |
| 2:b:5005:TRP:CZ2  | 28:l:6061:MGE:C2A  | 2.80                     | 0.43              |
| 2:b:5463:PHE:CD2  | 29:b:6058:DGD:HAV1 | 2.54                     | 0.43              |
| 3:c:5042:LEU:CG   | 3:c:5049:LEU:HD11  | 2.49                     | 0.43              |
| 3:c:5145:SER:O    | 3:c:5147:PHE:N     | 2.52                     | 0.43              |
| 3:c:5327:ASN:ND2  | 3:c:5330:SER:N     | 2.67                     | 0.43              |
| 3:c:5342:MET:HG2  | 3:c:5343:ARG:N     | 2.34                     | 0.43              |
| 22:c:6035:CLA:CBB | 22:k:6034:CLA:CHB  | 2.96                     | 0.43              |
| 4:d:5145:ALA:HA   | 4:d:5276:VAL:HG11  | 2.00                     | 0.43              |
| 4:d:5176:ALA:O    | 4:d:5179:PHE:N     | 2.52                     | 0.43              |
| 4:d:5191:TRP:O    | 4:d:5193:LEU:N     | 2.52                     | 0.43              |
| 5:e:5077:GLU:C    | 5:e:5079:PHE:N     | 2.74                     | 0.43              |
| 6:f:5016:PHE:CZ   | 31:f:6040:HEM:HBD2 | 2.54                     | 0.43              |
| 7:h:5017:GLU:O    | 7:h:5017:GLU:HG2   | 2.19                     | 0.43              |
| 9:j:5010:LEU:CD2  | 9:j:5011:TRP:H     | 2.31                     | 0.43              |
| 10:k:5024:VAL:O   | 10:k:5025:LEU:C    | 2.62                     | 0.43              |
| 25:k:6051:BCR:C23 | 25:k:6051:BCR:H392 | 2.48                     | 0.43              |
| 11:l:5025:LEU:HB3 | 14:t:5013:ILE:HG12 | 2.01                     | 0.43              |
| 13:o:5142:ILE:HA  | 13:o:5143:PRO:HD3  | 1.78                     | 0.43              |
| 13:o:5245:GLN:C   | 13:o:5246:LEU:HD23 | 2.43                     | 0.43              |
| 25:t:1046:BCR:C23 | 25:t:1046:BCR:C40  | 2.92                     | 0.43              |
| 16:v:5045:ILE:O   | 16:v:5045:ILE:HG22 | 2.19                     | 0.43              |
| 20:z:5029:SER:HB2 | 20:z:5031:GLN:HE21 | 1.83                     | 0.43              |
| 1:A:38:ILE:O      | 1:A:42:LEU:HD23    | 2.18                     | 0.43              |
| 1:A:63:ILE:HG12   | 1:A:65:GLU:N       | 2.34                     | 0.43              |
| 1:A:295:PHE:HD2   | 3:C:291:TRP:CE2    | 2.37                     | 0.43              |
| 22:A:1006:CLA:CAA | 29:C:1057:DGD:HBN2 | 2.48                     | 0.43              |
| 2:B:3:LEU:O       | 11:L:10:VAL:HA     | 2.19                     | 0.43              |
| 2:B:181:VAL:HG11  | 2:B:196:GLY:HA2    | 1.98                     | 0.43              |
| 2:B:291:SER:O     | 2:B:296:ALA:HB3    | 2.18                     | 0.43              |
| 2:B:447:PRO:O     | 2:B:448:ARG:C      | 2.61                     | 0.43              |
| 22:B:1011:CLA:CGD | 22:B:1011:CLA:HAA2 | 2.48                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1023:CLA:H111 | 22:B:1023:CLA:H142 | 1.61                     | 0.43              |
| 3:C:139:THR:HG23   | 3:C:142:GLU:CG     | 2.48                     | 0.43              |
| 3:C:327:ASN:HD21   | 3:C:331:ALA:N      | 2.17                     | 0.43              |
| 3:C:327:ASN:ND2    | 3:C:330:SER:N      | 2.67                     | 0.43              |
| 22:C:1035:CLA:H143 | 22:C:1035:CLA:H112 | 1.79                     | 0.43              |
| 4:D:111:TRP:O      | 4:D:112:THR:C      | 2.61                     | 0.43              |
| 6:F:22:ALA:O       | 6:F:23:VAL:C       | 2.62                     | 0.43              |
| 7:H:27:THR:HG22    | 22:H:1017:CLA:HMD2 | 2.01                     | 0.43              |
| 25:T:6048:BCR:H23C | 2:b:5109:LEU:HB3   | 2.01                     | 0.43              |
| 16:V:107:THR:C     | 16:V:109:ASP:H     | 2.26                     | 0.43              |
| 18:Y:43:ARG:HH21   | 18:Y:44:GLY:N      | 2.14                     | 0.43              |
| 1:a:5089:ILE:HD13  | 1:a:5094:TYR:CG    | 2.53                     | 0.43              |
| 1:a:5113:GLN:CA    | 1:a:5116:ILE:HG22  | 2.48                     | 0.43              |
| 1:a:5113:GLN:HB3   | 1:a:5117:PHE:CE1   | 2.54                     | 0.43              |
| 1:a:5133:LEU:HB3   | 4:d:5252:PHE:HE2   | 1.84                     | 0.43              |
| 1:a:5183:MET:O     | 1:a:5186:PHE:N     | 2.52                     | 0.43              |
| 1:a:5197:PHE:O     | 1:a:5198:HIS:C     | 2.61                     | 0.43              |
| 1:a:5279:ARG:NH2   | 1:a:5283:VAL:HG22  | 2.34                     | 0.43              |
| 1:a:5310:LYS:HG2   | 16:v:5151:ILE:CG2  | 2.46                     | 0.43              |
| 2:b:5016:PRO:CG    | 2:b:5133:LEU:HD13  | 2.46                     | 0.43              |
| 2:b:5055:MET:CE    | 2:b:5080:ILE:CG2   | 2.93                     | 0.43              |
| 2:b:5067:ALA:O     | 2:b:5068:ARG:C     | 2.60                     | 0.43              |
| 2:b:5238:LEU:N     | 22:b:6020:CLA:CMD  | 2.82                     | 0.43              |
| 2:b:5452:THR:HB    | 4:d:5291:LEU:CD1   | 2.48                     | 0.43              |
| 25:b:6047:BCR:C30  | 25:b:6047:BCR:C37  | 2.61                     | 0.43              |
| 3:c:5123:ALA:HA    | 25:k:6052:BCR:C14  | 2.48                     | 0.43              |
| 3:c:5139:THR:HG23  | 3:c:5139:THR:O     | 2.18                     | 0.43              |
| 3:c:5284:PHE:HB3   | 29:c:6055:DGD:HB81 | 2.00                     | 0.43              |
| 3:c:5327:ASN:HD21  | 3:c:5331:ALA:N     | 2.17                     | 0.43              |
| 22:c:6026:CLA:H92  | 22:c:6026:CLA:H61  | 1.63                     | 0.43              |
| 22:c:6035:CLA:H61  | 25:k:6052:BCR:H401 | 1.99                     | 0.43              |
| 4:d:5090:LEU:O     | 22:d:6008:CLA:HED1 | 2.18                     | 0.43              |
| 4:d:5263:ASN:OD1   | 4:d:5264:LYS:N     | 2.52                     | 0.43              |
| 4:d:5297:ASP:OD1   | 4:d:5298:PHE:N     | 2.27                     | 0.43              |
| 22:d:6008:CLA:H41  | 22:d:6008:CLA:H61  | 1.64                     | 0.43              |
| 7:h:5031:MET:SD    | 22:h:6017:CLA:CAA  | 3.04                     | 0.43              |
| 25:h:6049:BCR:C8   | 25:h:6049:BCR:C32  | 2.95                     | 0.43              |
| 13:o:5188:ARG:NH1  | 13:o:5188:ARG:CB   | 2.76                     | 0.43              |
| 15:u:5041:LEU:HD11 | 15:u:5074:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:147:TYR:CE2    | 23:A:1038:PHO:HAA1 | 2.53                     | 0.43              |
| 1:A:329:GLU:O      | 1:A:332:HIS:ND1    | 2.47                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1021:CLA:HBC3 | 25:B:1047:BCR:C34  | 2.49                     | 0.43              |
| 3:C:46:SER:O       | 3:C:47:GLY:C       | 2.59                     | 0.43              |
| 3:C:127:PHE:C      | 3:C:130:VAL:HG12   | 2.42                     | 0.43              |
| 3:C:322:GLN:NE2    | 3:C:381:LYS:HG2    | 2.34                     | 0.43              |
| 22:C:1028:CLA:H62  | 29:C:1057:DGD:HA42 | 2.01                     | 0.43              |
| 22:C:1037:CLA:H142 | 22:C:1037:CLA:C10  | 2.48                     | 0.43              |
| 4:D:39:PRO:CB      | 22:D:1008:CLA:CBB  | 2.97                     | 0.43              |
| 7:H:30:LEU:CA      | 7:H:33:VAL:HG22    | 2.48                     | 0.43              |
| 10:K:18:PHE:CD1    | 10:K:18:PHE:N      | 2.86                     | 0.43              |
| 10:K:24:VAL:O      | 10:K:25:LEU:C      | 2.62                     | 0.43              |
| 22:K:1034:CLA:H41  | 22:K:1034:CLA:C8   | 2.48                     | 0.43              |
| 17:X:11:THR:O      | 17:X:11:THR:CG2    | 2.65                     | 0.43              |
| 17:X:13:THR:HG22   | 17:X:14:PRO:HD2    | 2.00                     | 0.43              |
| 20:Z:29:SER:HB2    | 20:Z:31:GLN:HE21   | 1.83                     | 0.43              |
| 1:a:5131:TRP:CE3   | 1:a:5132:GLU:N     | 2.87                     | 0.43              |
| 1:a:5201:GLY:C     | 1:a:5203:ALA:H     | 2.27                     | 0.43              |
| 1:a:5310:LYS:HE2   | 16:v:5151:ILE:HG22 | 2.00                     | 0.43              |
| 2:b:5103:LEU:HD12  | 2:b:5103:LEU:C     | 2.44                     | 0.43              |
| 2:b:5307:GLU:O     | 2:b:5308:LYS:C     | 2.61                     | 0.43              |
| 2:b:5341:LYS:HD2   | 2:b:5429:ILE:HG22  | 2.00                     | 0.43              |
| 2:b:5460:LEU:HD23  | 2:b:5460:LEU:C     | 2.43                     | 0.43              |
| 22:b:6023:CLA:CMB  | 22:b:6023:CLA:HBB1 | 2.48                     | 0.43              |
| 3:c:5146:PHE:O     | 3:c:5147:PHE:HB2   | 2.19                     | 0.43              |
| 3:c:5267:SER:O     | 3:c:5268:GLY:C     | 2.59                     | 0.43              |
| 3:c:5436:PHE:HD2   | 3:c:5436:PHE:HA    | 1.72                     | 0.43              |
| 22:c:6032:CLA:H121 | 10:k:5033:PHE:HZ   | 1.82                     | 0.43              |
| 4:d:5217:THR:CG2   | 4:d:5218:VAL:N     | 2.81                     | 0.43              |
| 5:e:5018:ARG:HG2   | 5:e:5022:ILE:HD11  | 2.01                     | 0.43              |
| 8:i:5025:SER:O     | 8:i:5026:GLY:O     | 2.36                     | 0.43              |
| 13:o:5079:LYS:HB2  | 13:o:5091:PHE:CE2  | 2.53                     | 0.43              |
| 13:o:5092:VAL:HG12 | 13:o:5093:PRO:HD2  | 2.00                     | 0.43              |
| 13:o:5104:LEU:CD1  | 13:o:5107:ILE:HD11 | 2.49                     | 0.43              |
| 13:o:5266:TYR:CG   | 13:o:5267:ALA:N    | 2.86                     | 0.43              |
| 16:v:5126:ILE:O    | 16:v:5128:PRO:HD3  | 2.18                     | 0.43              |
| 20:z:5033:TRP:O    | 20:z:5037:LYS:HB3  | 2.19                     | 0.43              |
| 2:B:24:LEU:HA      | 22:B:1023:CLA:HED3 | 2.01                     | 0.43              |
| 2:B:62:VAL:HG11    | 22:B:1013:CLA:HED2 | 2.00                     | 0.43              |
| 2:B:135:LEU:HB2    | 2:B:136:PRO:HD3    | 2.01                     | 0.43              |
| 2:B:298:LEU:HG     | 2:B:402:TYR:CD2    | 2.53                     | 0.43              |
| 2:B:338:GLN:HE21   | 2:B:338:GLN:CA     | 2.17                     | 0.43              |
| 22:B:1009:CLA:CBA  | 22:B:1009:CLA:O2D  | 2.60                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:82:TYR:CD2     | 3:C:302:TYR:O      | 2.72                     | 0.43              |
| 3:C:100:GLY:O      | 3:C:102:GLY:O      | 2.36                     | 0.43              |
| 3:C:163:PHE:O      | 3:C:166:ILE:HG12   | 2.19                     | 0.43              |
| 3:C:172:ALA:H      | 22:C:1025:CLA:HBC2 | 1.76                     | 0.43              |
| 3:C:397:THR:O      | 3:C:399:ALA:N      | 2.52                     | 0.43              |
| 22:C:1029:CLA:HMD1 | 22:C:1031:CLA:CAB  | 2.38                     | 0.43              |
| 4:D:145:ALA:HB2    | 4:D:272:LEU:HD12   | 2.00                     | 0.43              |
| 4:D:253:TRP:O      | 4:D:254:SER:C      | 2.61                     | 0.43              |
| 4:D:263:ASN:OD1    | 4:D:264:LYS:N      | 2.52                     | 0.43              |
| 13:O:36:ILE:O      | 13:O:36:ILE:CG2    | 2.66                     | 0.43              |
| 13:O:74:THR:HG22   | 13:O:263:GLY:HA2   | 2.00                     | 0.43              |
| 13:O:142:ILE:HA    | 13:O:143:PRO:HD3   | 1.78                     | 0.43              |
| 13:O:163:THR:C     | 13:O:165:SER:H     | 2.26                     | 0.43              |
| 13:O:266:TYR:CG    | 13:O:267:ALA:N     | 2.86                     | 0.43              |
| 16:V:101:TYR:CE2   | 31:V:1041:HEM:HAA1 | 2.54                     | 0.43              |
| 1:a:5199:GLN:HE21  | 1:a:5199:GLN:HB3   | 1.47                     | 0.43              |
| 2:b:5034:ALA:O     | 2:b:5035:GLY:C     | 2.62                     | 0.43              |
| 2:b:5037:MET:O     | 2:b:5038:ALA:C     | 2.62                     | 0.43              |
| 2:b:5098:LEU:O     | 2:b:5098:LEU:HD22  | 2.19                     | 0.43              |
| 2:b:5347:ARG:HG2   | 2:b:5347:ARG:HH11  | 1.83                     | 0.43              |
| 2:b:5468:TRP:CE2   | 22:b:6019:CLA:HED2 | 2.53                     | 0.43              |
| 22:b:6018:CLA:HHC  | 22:b:6018:CLA:CBB  | 2.20                     | 0.43              |
| 3:c:5274:TYR:CE2   | 22:c:6031:CLA:HMC1 | 2.54                     | 0.43              |
| 4:d:5085:MET:HA    | 5:e:5069:ARG:HB3   | 2.00                     | 0.43              |
| 4:d:5226:GLY:CA    | 4:d:5234:ALA:CB    | 2.92                     | 0.43              |
| 4:d:5312:GLU:CD    | 13:o:5185:PRO:HB3  | 2.43                     | 0.43              |
| 8:i:5014:PHE:CE1   | 8:i:5018:LEU:HD12  | 2.42                     | 0.43              |
| 25:k:6052:BCR:C8   | 25:k:6052:BCR:H331 | 2.49                     | 0.43              |
| 13:o:5037:VAL:O    | 13:o:5037:VAL:HG13 | 2.19                     | 0.43              |
| 13:o:5045:CYS:CB   | 13:o:5046:PRO:HD2  | 2.32                     | 0.43              |
| 13:o:5115:SER:O    | 13:o:5116:ASP:CG   | 2.62                     | 0.43              |
| 13:o:5145:LEU:HD12 | 13:o:5145:LEU:HA   | 1.80                     | 0.43              |
| 13:o:5175:PRO:HG2  | 13:o:5176:SER:N    | 2.34                     | 0.43              |
| 16:v:5047:LEU:HD21 | 16:v:5051:GLN:HB2  | 2.01                     | 0.43              |
| 1:A:133:LEU:HD23   | 4:D:252:PHE:CD2    | 2.53                     | 0.42              |
| 1:A:305:SER:HB3    | 3:C:415:ASN:HD21   | 1.84                     | 0.42              |
| 2:B:34:ALA:O       | 2:B:35:GLY:C       | 2.62                     | 0.42              |
| 2:B:98:LEU:O       | 2:B:98:LEU:HD22    | 2.19                     | 0.42              |
| 2:B:98:LEU:C       | 2:B:98:LEU:CD1     | 2.87                     | 0.42              |
| 2:B:359:MET:HA     | 2:B:360:PRO:HD2    | 1.85                     | 0.42              |
| 3:C:128:GLY:N      | 22:C:1037:CLA:HAC2 | 2.34                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:321:ASP:OD2   | 3:C:321:ASP:N      | 2.52                     | 0.42              |
| 22:C:1027:CLA:H62 | 22:C:1027:CLA:H41  | 1.60                     | 0.42              |
| 22:C:1036:CLA:H42 | 22:C:1036:CLA:O2A  | 2.19                     | 0.42              |
| 4:D:96:GLU:CD     | 4:D:96:GLU:H       | 2.26                     | 0.42              |
| 4:D:195:PRO:O     | 4:D:196:PHE:C      | 2.61                     | 0.42              |
| 4:D:276:VAL:HG23  | 4:D:277:THR:H      | 1.83                     | 0.42              |
| 6:F:32:PHE:HD1    | 6:F:32:PHE:C       | 2.27                     | 0.42              |
| 12:M:33:GLN:C     | 12:M:35:SER:H      | 2.26                     | 0.42              |
| 13:O:227:VAL:HG13 | 13:O:237:ILE:HG13  | 2.00                     | 0.42              |
| 16:V:105:PRO:HD3  | 16:V:120:SER:HB3   | 2.01                     | 0.42              |
| 1:a:5147:TYR:CE2  | 23:a:6038:PHO:HAA1 | 2.53                     | 0.42              |
| 1:a:5160:ILE:HD13 | 3:c:5431:PHE:HE1   | 1.80                     | 0.42              |
| 1:a:5267:ASN:O    | 1:a:5268:SER:C     | 2.62                     | 0.42              |
| 1:a:5271:LEU:C    | 1:a:5273:PHE:N     | 2.76                     | 0.42              |
| 1:a:5281:VAL:O    | 1:a:5284:TRP:HB2   | 2.19                     | 0.42              |
| 24:a:6043:PQ9:C45 | 24:a:6043:PQ9:C40  | 2.96                     | 0.42              |
| 24:a:6043:PQ9:H37 | 24:a:6043:PQ9:H311 | 2.01                     | 0.42              |
| 2:b:5047:PRO:O    | 2:b:5048:SER:C     | 2.61                     | 0.42              |
| 2:b:5068:ARG:HE   | 2:b:5264:PRO:HD3   | 1.84                     | 0.42              |
| 2:b:5099:ALA:C    | 2:b:5101:ILE:N     | 2.76                     | 0.42              |
| 2:b:5159:THR:HG22 | 2:b:5199:VAL:HG11  | 2.01                     | 0.42              |
| 2:b:5191:ASN:O    | 2:b:5194:ASN:N     | 2.52                     | 0.42              |
| 2:b:5228:ALA:C    | 2:b:5230:ARG:H     | 2.27                     | 0.42              |
| 2:b:5346:PHE:HE1  | 2:b:5421:ALA:HB2   | 1.84                     | 0.42              |
| 22:b:6011:CLA:CGD | 22:b:6011:CLA:HAA2 | 2.48                     | 0.42              |
| 22:b:6015:CLA:C20 | 11:l:5027:LEU:HD13 | 2.49                     | 0.42              |
| 3:c:5081:MET:SD   | 3:c:5089:ILE:HG22  | 2.59                     | 0.42              |
| 3:c:5119:LEU:HD11 | 25:k:6052:BCR:C34  | 2.48                     | 0.42              |
| 3:c:5154:LYS:HE3  | 3:c:5261:ARG:HE    | 1.83                     | 0.42              |
| 3:c:5379:LYS:O    | 3:c:5380:ILE:C     | 2.61                     | 0.42              |
| 4:d:5127:LEU:O    | 4:d:5130:PHE:HB2   | 2.19                     | 0.42              |
| 4:d:5197:HIS:ND1  | 4:d:5197:HIS:C     | 2.76                     | 0.42              |
| 4:d:5230:SER:C    | 4:d:5232:PHE:N     | 2.74                     | 0.42              |
| 4:d:5236:ASN:OD1  | 4:d:5239:GLN:O     | 2.37                     | 0.42              |
| 5:e:5048:GLY:O    | 5:e:5049:THR:C     | 2.61                     | 0.42              |
| 6:f:5032:PHE:HD1  | 6:f:5032:PHE:C     | 2.27                     | 0.42              |
| 7:h:5030:LEU:CA   | 7:h:5033:VAL:HG22  | 2.48                     | 0.42              |
| 22:k:6034:CLA:H41 | 22:k:6034:CLA:C8   | 2.48                     | 0.42              |
| 12:m:5031:SER:HA  | 12:m:5035:SER:O    | 2.19                     | 0.42              |
| 13:o:5234:THR:HB  | 13:o:5236:GLU:HG3  | 2.01                     | 0.42              |
| 14:t:5022:PHE:N   | 14:t:5022:PHE:HD1  | 2.17                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:58:VAL:CG2     | 1:A:83:VAL:HG23    | 2.49                     | 0.42              |
| 1:A:113:GLN:CA     | 1:A:116:ILE:HG22   | 2.48                     | 0.42              |
| 1:A:267:ASN:O      | 1:A:268:SER:C      | 2.62                     | 0.42              |
| 1:A:289:GLY:O      | 1:A:293:MET:HE3    | 2.18                     | 0.42              |
| 1:A:318:ALA:HA     | 1:A:321:ILE:HD12   | 2.00                     | 0.42              |
| 22:A:1006:CLA:H161 | 25:D:1050:BCR:C27  | 2.44                     | 0.42              |
| 2:B:6:TYR:O        | 22:B:1019:CLA:CBA  | 2.66                     | 0.42              |
| 2:B:13:ILE:HD12    | 2:B:234:ILE:HG23   | 2.01                     | 0.42              |
| 2:B:30:VAL:O       | 2:B:33:TRP:N       | 2.52                     | 0.42              |
| 2:B:68:ARG:HE      | 2:B:264:PRO:HD3    | 1.84                     | 0.42              |
| 2:B:99:ALA:C       | 2:B:101:ILE:N      | 2.76                     | 0.42              |
| 2:B:237:VAL:HB     | 22:B:1020:CLA:HMD2 | 1.99                     | 0.42              |
| 2:B:284:ILE:HD11   | 2:B:309:LEU:HG     | 2.01                     | 0.42              |
| 22:B:1015:CLA:C20  | 11:L:27:LEU:HD13   | 2.49                     | 0.42              |
| 3:C:54:VAL:HG12    | 3:C:125:LEU:O      | 2.19                     | 0.42              |
| 3:C:89:ILE:HG23    | 3:C:111:PHE:HE2    | 1.80                     | 0.42              |
| 3:C:130:VAL:CG2    | 22:C:1035:CLA:H102 | 2.49                     | 0.42              |
| 3:C:151:TRP:O      | 3:C:152:LYS:C      | 2.62                     | 0.42              |
| 22:C:1031:CLA:OBD  | 22:C:1033:CLA:C15  | 2.68                     | 0.42              |
| 22:C:1035:CLA:CBB  | 22:K:1034:CLA:CHB  | 2.96                     | 0.42              |
| 4:D:120:PHE:CD1    | 4:D:123:ILE:HD12   | 2.55                     | 0.42              |
| 4:D:127:LEU:O      | 4:D:130:PHE:HB2    | 2.19                     | 0.42              |
| 5:E:13:ILE:HG13    | 5:E:13:ILE:O       | 2.18                     | 0.42              |
| 7:H:35:MET:SD      | 22:H:1017:CLA:H42  | 2.59                     | 0.42              |
| 10:K:12:PRO:HB3    | 20:Z:62:VAL:HG21   | 2.00                     | 0.42              |
| 22:K:1034:CLA:CGA  | 22:K:1034:CLA:C1A  | 2.97                     | 0.42              |
| 12:M:31:SER:HA     | 12:M:35:SER:O      | 2.19                     | 0.42              |
| 12:M:32:GLN:NE2    | 12:m:5031:SER:O    | 2.52                     | 0.42              |
| 13:O:265:PHE:CD1   | 13:O:265:PHE:C     | 2.94                     | 0.42              |
| 17:X:12:ILE:O      | 17:X:12:ILE:CG1    | 2.67                     | 0.42              |
| 1:a:5060:ILE:O     | 1:a:5061:ASP:O     | 2.37                     | 0.42              |
| 1:a:5120:LEU:HD13  | 1:a:5120:LEU:C     | 2.44                     | 0.42              |
| 1:a:5285:PHE:O     | 1:a:5288:LEU:HB2   | 2.19                     | 0.42              |
| 22:a:6003:CLA:C14  | 23:a:6038:PHO:C7   | 2.97                     | 0.42              |
| 2:b:5015:ASP:CG    | 2:b:5018:ARG:HG3   | 2.43                     | 0.42              |
| 2:b:5095:GLY:O     | 2:b:5099:ALA:CB    | 2.67                     | 0.42              |
| 2:b:5264:PRO:HG3   | 2:b:5267:LEU:HD12  | 1.99                     | 0.42              |
| 2:b:5347:ARG:O     | 2:b:5398:THR:HG22  | 2.19                     | 0.42              |
| 2:b:5437:LEU:O     | 2:b:5438:ASN:HB3   | 2.19                     | 0.42              |
| 3:c:5131:TYR:C     | 3:c:5133:ALA:N     | 2.77                     | 0.42              |
| 3:c:5162:GLY:HA2   | 3:c:5248:GLY:HA2   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6027:CLA:H62  | 22:c:6027:CLA:H41  | 1.60                     | 0.42              |
| 22:c:6037:CLA:HHC  | 22:c:6037:CLA:CBB  | 2.20                     | 0.42              |
| 4:d:5088:SER:CA    | 7:h:5050:ASN:HD21  | 2.03                     | 0.42              |
| 4:d:5191:TRP:CD1   | 4:d:5197:HIS:CD2   | 3.07                     | 0.42              |
| 22:d:6008:CLA:H61  | 22:d:6008:CLA:H101 | 1.69                     | 0.42              |
| 9:j:5018:GLY:HA3   | 25:k:6051:BCR:H371 | 2.01                     | 0.42              |
| 12:m:5008:PHE:O    | 12:m:5012:ALA:CB   | 2.67                     | 0.42              |
| 13:o:5069:LEU:HD12 | 13:o:5069:LEU:C    | 2.44                     | 0.42              |
| 13:o:5231:ASP:CB   | 13:o:5234:THR:OG1  | 2.65                     | 0.42              |
| 1:A:120:LEU:HD13   | 1:A:120:LEU:C      | 2.44                     | 0.42              |
| 1:A:201:GLY:C      | 1:A:203:ALA:H      | 2.27                     | 0.42              |
| 1:A:219:VAL:CB     | 4:D:268:HIS:HB3    | 2.49                     | 0.42              |
| 1:A:280:VAL:CG2    | 4:D:212:ALA:HB1    | 2.49                     | 0.42              |
| 1:A:290:ILE:HG12   | 22:A:1003:CLA:OBD  | 2.19                     | 0.42              |
| 1:A:340:PRO:CD     | 15:U:103:TYR:HE2   | 2.32                     | 0.42              |
| 2:B:89:GLY:O       | 2:B:90:PHE:C       | 2.59                     | 0.42              |
| 2:B:139:PHE:CZ     | 22:H:1017:CLA:CMB  | 3.02                     | 0.42              |
| 2:B:346:PHE:N      | 2:B:346:PHE:CD2    | 2.87                     | 0.42              |
| 2:B:347:ARG:O      | 2:B:398:THR:HG22   | 2.20                     | 0.42              |
| 22:B:1020:CLA:H8   | 22:B:1020:CLA:H51  | 1.91                     | 0.42              |
| 29:B:1058:DGD:HBV2 | 4:D:287:VAL:HG22   | 2.01                     | 0.42              |
| 3:C:164:HIS:CA     | 3:C:167:VAL:HB     | 2.47                     | 0.42              |
| 3:C:397:THR:HG1    | 3:C:398:HIS:N      | 2.17                     | 0.42              |
| 22:C:1033:CLA:C9   | 22:C:1036:CLA:CAA  | 2.97                     | 0.42              |
| 22:C:1035:CLA:HBA1 | 22:C:1035:CLA:H3A  | 1.88                     | 0.42              |
| 22:C:1037:CLA:H72  | 22:C:1037:CLA:H111 | 1.60                     | 0.42              |
| 29:C:1056:DGD:HB32 | 29:C:1057:DGD:HA31 | 2.01                     | 0.42              |
| 4:D:183:LEU:O      | 4:D:184:PHE:C      | 2.62                     | 0.42              |
| 4:D:191:TRP:CD1    | 4:D:197:HIS:CD2    | 3.07                     | 0.42              |
| 24:D:1042:PQ9:H27  | 24:D:1042:PQ9:H312 | 1.57                     | 0.42              |
| 6:F:15:ILE:HD12    | 31:F:1040:HEM:CMD  | 2.49                     | 0.42              |
| 6:F:16:PHE:CZ      | 31:F:1040:HEM:HBD2 | 2.54                     | 0.42              |
| 9:J:29:PHE:O       | 9:J:30:TYR:C       | 2.60                     | 0.42              |
| 11:L:29:LEU:C      | 11:L:29:LEU:CD1    | 2.90                     | 0.42              |
| 13:O:41:LEU:C      | 13:O:43:ASN:N      | 2.77                     | 0.42              |
| 13:O:92:VAL:CG1    | 13:O:93:PRO:CD     | 2.98                     | 0.42              |
| 25:T:6046:BCR:C33  | 25:T:6046:BCR:C8   | 2.72                     | 0.42              |
| 15:U:78:ASN:O      | 15:U:79:LEU:C      | 2.61                     | 0.42              |
| 16:V:138:LEU:HA    | 16:V:138:LEU:HD23  | 1.79                     | 0.42              |
| 20:Z:58:ASN:C      | 20:Z:60:PHE:N      | 2.77                     | 0.42              |
| 1:a:5081:ALA:CA    | 1:a:5175:GLY:HA3   | 2.49                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5259:ILE:HD13  | 24:a:6043:PQ9:C24  | 2.38                     | 0.42              |
| 22:a:6003:CLA:H141 | 23:a:6038:PHO:C8   | 2.45                     | 0.42              |
| 22:a:6006:CLA:H161 | 25:d:6050:BCR:C27  | 2.44                     | 0.42              |
| 2:b:5192:PRO:HG3   | 7:h:5049:TYR:CD1   | 2.55                     | 0.42              |
| 2:b:5298:LEU:HG    | 2:b:5402:TYR:CD2   | 2.54                     | 0.42              |
| 2:b:5321:LYS:HZ3   | 2:b:5321:LYS:HA    | 1.85                     | 0.42              |
| 22:b:6022:CLA:C9   | 22:b:6022:CLA:C13  | 2.78                     | 0.42              |
| 3:c:5062:PHE:HZ    | 10:k:5028:ILE:HB   | 1.84                     | 0.42              |
| 3:c:5100:GLY:O     | 3:c:5102:GLY:O     | 2.36                     | 0.42              |
| 3:c:5128:GLY:N     | 22:c:6037:CLA:HAC2 | 2.34                     | 0.42              |
| 3:c:5130:VAL:CG2   | 22:c:6035:CLA:H102 | 2.49                     | 0.42              |
| 3:c:5220:GLY:C     | 3:c:5221:GLU:HG3   | 2.44                     | 0.42              |
| 3:c:5276:LEU:HD22  | 3:c:5441:HIS:N     | 2.34                     | 0.42              |
| 22:c:6028:CLA:HMC2 | 22:k:6034:CLA:CED  | 2.48                     | 0.42              |
| 22:c:6029:CLA:C4D  | 22:c:6029:CLA:C1   | 2.85                     | 0.42              |
| 4:d:5039:PRO:CB    | 22:d:6008:CLA:CBB  | 2.97                     | 0.42              |
| 4:d:5048:TRP:CD1   | 23:d:6039:PHO:H162 | 2.53                     | 0.42              |
| 4:d:5068:LEU:CA    | 6:f:5040:MET:SD    | 3.06                     | 0.42              |
| 5:e:5027:ILE:HB    | 5:e:5028:PRO:CD    | 2.44                     | 0.42              |
| 7:h:5035:MET:SD    | 22:h:6017:CLA:H42  | 2.59                     | 0.42              |
| 7:h:5048:ILE:CA    | 7:h:5053:LEU:HB3   | 2.47                     | 0.42              |
| 22:h:6017:CLA:H93  | 22:h:6017:CLA:H62  | 1.59                     | 0.42              |
| 11:l:5019:LEU:N    | 11:l:5019:LEU:HD23 | 2.34                     | 0.42              |
| 13:o:5227:VAL:HG13 | 13:o:5237:ILE:HG13 | 2.00                     | 0.42              |
| 15:u:5031:ASN:ND2  | 15:u:5031:ASN:C    | 2.76                     | 0.42              |
| 15:u:5036:ILE:HA   | 15:u:5042:TYR:HB2  | 2.00                     | 0.42              |
| 20:z:5005:PHE:O    | 20:z:5008:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:62:GLY:CA      | 1:A:87:ASN:HB2     | 2.46                     | 0.42              |
| 1:A:91:LEU:C       | 1:A:92:HIS:O       | 2.59                     | 0.42              |
| 1:A:140:ARG:HB2    | 4:D:220:ASN:HA     | 2.01                     | 0.42              |
| 1:A:183:MET:O      | 1:A:186:PHE:N      | 2.52                     | 0.42              |
| 1:A:281:VAL:O      | 1:A:284:TRP:HB2    | 2.19                     | 0.42              |
| 1:A:309:ALA:O      | 1:A:311:GLY:N      | 2.51                     | 0.42              |
| 1:A:310:LYS:HE2    | 16:V:151:ILE:HG22  | 2.00                     | 0.42              |
| 22:A:1006:CLA:H2   | 22:A:1006:CLA:H61  | 1.68                     | 0.42              |
| 2:B:37:MET:O       | 2:B:38:ALA:C       | 2.62                     | 0.42              |
| 2:B:95:GLY:O       | 2:B:99:ALA:CB      | 2.67                     | 0.42              |
| 2:B:159:THR:HG22   | 2:B:199:VAL:HG11   | 2.01                     | 0.42              |
| 2:B:268:PHE:CD1    | 2:B:268:PHE:N      | 2.88                     | 0.42              |
| 2:B:437:LEU:O      | 2:B:438:ASN:HB3    | 2.19                     | 0.42              |
| 22:B:1018:CLA:H112 | 22:B:1018:CLA:H142 | 1.64                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1022:CLA:C9   | 22:B:1022:CLA:CB   | 2.62                     | 0.42              |
| 29:B:1058:DGD:HG11 | 7:H:50:ASN:HD22    | 1.84                     | 0.42              |
| 3:C:82:TYR:HD1     | 3:C:419:PHE:HE2    | 1.66                     | 0.42              |
| 3:C:117:VAL:HG21   | 22:C:1027:CLA:C4   | 2.49                     | 0.42              |
| 3:C:162:GLY:HA2    | 3:C:248:GLY:HA2    | 2.01                     | 0.42              |
| 22:C:1028:CLA:HMC2 | 22:K:1034:CLA:CED  | 2.48                     | 0.42              |
| 4:D:14:TRP:O       | 4:D:17:ILE:CG1     | 2.67                     | 0.42              |
| 4:D:89:LEU:CD1     | 7:H:50:ASN:OD1     | 2.62                     | 0.42              |
| 4:D:312:GLU:CD     | 13:O:185:PRO:HB3   | 2.43                     | 0.42              |
| 22:D:1005:CLA:HBD  | 22:D:1005:CLA:HAA1 | 2.01                     | 0.42              |
| 5:E:22:ILE:O       | 5:E:25:ILE:HG13    | 2.18                     | 0.42              |
| 10:K:35:LEU:C      | 10:K:37:PHE:N      | 2.76                     | 0.42              |
| 13:O:52:ALA:CB     | 13:O:229:LYS:HA    | 2.50                     | 0.42              |
| 13:O:115:SER:O     | 13:O:116:ASP:CG    | 2.62                     | 0.42              |
| 13:O:260:LYS:O     | 13:O:261:ILE:HD13  | 2.19                     | 0.42              |
| 16:V:108:TYR:O     | 16:V:108:TYR:CD2   | 2.72                     | 0.42              |
| 20:Z:45:GLY:O      | 20:Z:49:ALA:CB     | 2.67                     | 0.42              |
| 1:a:5059:ASP:OD2   | 1:a:5059:ASP:N     | 2.51                     | 0.42              |
| 1:a:5215:HIS:CD2   | 1:a:5275:LEU:CD1   | 3.00                     | 0.42              |
| 2:b:5030:VAL:O     | 2:b:5033:TRP:N     | 2.52                     | 0.42              |
| 2:b:5121:GLU:HB3   | 7:h:5004:ARG:HA    | 2.02                     | 0.42              |
| 2:b:5135:LEU:HB2   | 2:b:5136:PRO:HD3   | 2.01                     | 0.42              |
| 22:b:6022:CLA:C14  | 22:b:6022:CLA:C10  | 2.71                     | 0.42              |
| 29:b:6058:DGD:HBV2 | 4:d:5287:VAL:HG22  | 2.01                     | 0.42              |
| 3:c:5082:TYR:CD2   | 3:c:5302:TYR:O     | 2.72                     | 0.42              |
| 3:c:5224:ILE:HG22  | 3:c:5289:PHE:CE1   | 2.54                     | 0.42              |
| 3:c:5298:PRO:O     | 3:c:5300:GLU:OE1   | 2.36                     | 0.42              |
| 3:c:5305:THR:O     | 3:c:5308:GLU:HB3   | 2.19                     | 0.42              |
| 3:c:5405:ASN:OD1   | 3:c:5405:ASN:C     | 2.62                     | 0.42              |
| 3:c:5438:LEU:HD13  | 3:c:5442:LEU:CD1   | 2.49                     | 0.42              |
| 22:c:6028:CLA:H62  | 22:c:6028:CLA:H41  | 1.42                     | 0.42              |
| 29:c:6056:DGD:C2B  | 29:c:6056:DGD:HG12 | 2.40                     | 0.42              |
| 29:c:6057:DGD:HB81 | 28:d:6059:MGE:C8B  | 2.24                     | 0.42              |
| 4:d:5141:TYR:O     | 4:d:5142:ASN:C     | 2.61                     | 0.42              |
| 4:d:5158:LEU:O     | 4:d:5162:LEU:CG    | 2.66                     | 0.42              |
| 4:d:5267:LEU:C     | 4:d:5267:LEU:CD2   | 2.91                     | 0.42              |
| 4:d:5277:THR:HG22  | 4:d:5278:GLY:N     | 2.34                     | 0.42              |
| 24:d:6042:PQ9:H32  | 24:d:6042:PQ9:H361 | 1.77                     | 0.42              |
| 5:e:5027:ILE:CD1   | 5:e:5027:ILE:N     | 2.82                     | 0.42              |
| 6:f:5043:ILE:O     | 9:j:5036:LEU:HG    | 2.20                     | 0.42              |
| 7:h:5005:THR:HB    | 7:h:5006:TRP:H     | 1.71                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:h:5028:THR:N     | 22:h:6017:CLA:OBD  | 2.52                     | 0.42              |
| 13:o:5172:PHE:CB   | 13:o:5221:GLY:HA3  | 2.48                     | 0.42              |
| 1:A:27:ARG:HG3     | 1:A:27:ARG:HH11    | 1.84                     | 0.42              |
| 1:A:102:LEU:HD12   | 1:A:102:LEU:C      | 2.43                     | 0.42              |
| 1:A:105:TRP:CD1    | 1:A:110:GLY:HA3    | 2.55                     | 0.42              |
| 1:A:113:GLN:HB3    | 1:A:117:PHE:CE1    | 2.54                     | 0.42              |
| 22:A:1003:CLA:C14  | 23:A:1038:PHO:C7   | 2.97                     | 0.42              |
| 22:A:1007:CLA:H112 | 22:A:1007:CLA:H72  | 1.53                     | 0.42              |
| 2:B:65:PHE:O       | 2:B:66:MET:C       | 2.63                     | 0.42              |
| 2:B:103:LEU:CG     | 2:B:104:SER:N      | 2.82                     | 0.42              |
| 2:B:109:LEU:HB3    | 25:B:1048:BCR:H23C | 2.01                     | 0.42              |
| 2:B:332:LYS:O      | 2:B:444:ARG:NH1    | 2.53                     | 0.42              |
| 22:B:1021:CLA:C12  | 28:B:1060:MGE:H132 | 2.50                     | 0.42              |
| 3:C:58:GLY:O       | 3:C:59:LEU:C       | 2.61                     | 0.42              |
| 3:C:89:ILE:N       | 3:C:90:PRO:CD      | 2.80                     | 0.42              |
| 3:C:305:THR:HG22   | 3:C:308:GLU:CB     | 2.41                     | 0.42              |
| 3:C:315:MET:HE2    | 3:C:319:ILE:CG1    | 2.50                     | 0.42              |
| 3:C:377:LEU:O      | 3:C:381:LYS:HB2    | 2.19                     | 0.42              |
| 4:D:191:TRP:O      | 4:D:193:LEU:N      | 2.52                     | 0.42              |
| 4:D:260:ALA:HA     | 24:D:1042:PQ9:H91  | 2.02                     | 0.42              |
| 7:H:3:ARG:HE       | 7:H:3:ARG:HB3      | 1.54                     | 0.42              |
| 7:H:17:GLU:O       | 7:H:17:GLU:HG2     | 2.19                     | 0.42              |
| 13:O:79:LYS:HB2    | 13:O:91:PHE:CE2    | 2.53                     | 0.42              |
| 13:O:254:HIS:H     | 13:O:254:HIS:CD2   | 2.38                     | 0.42              |
| 25:T:6046:BCR:C23  | 25:T:6046:BCR:C40  | 2.92                     | 0.42              |
| 15:U:31:ASN:ND2    | 15:U:31:ASN:C      | 2.76                     | 0.42              |
| 15:U:36:ILE:HG22   | 15:U:42:TYR:HB2    | 2.02                     | 0.42              |
| 18:Y:30:ILE:O      | 18:Y:30:ILE:CG1    | 2.67                     | 0.42              |
| 1:a:5091:LEU:C     | 1:a:5092:HIS:O     | 2.58                     | 0.42              |
| 1:a:5095:PRO:HD2   | 1:a:5098:GLU:HB2   | 2.00                     | 0.42              |
| 1:a:5309:ALA:C     | 1:a:5311:GLY:N     | 2.77                     | 0.42              |
| 22:a:6006:CLA:C9   | 22:d:6004:CLA:H152 | 2.46                     | 0.42              |
| 23:a:6038:PHO:H91  | 22:d:6005:CLA:C17  | 2.49                     | 0.42              |
| 26:a:6063:LHG:HC11 | 3:c:5447:ARG:HH12  | 1.85                     | 0.42              |
| 2:b:5052:LEU:CD1   | 2:b:5339:ALA:HA    | 2.49                     | 0.42              |
| 2:b:5099:ALA:O     | 2:b:5101:ILE:N     | 2.53                     | 0.42              |
| 2:b:5311:PHE:O     | 2:b:5311:PHE:HD2   | 2.03                     | 0.42              |
| 2:b:5389:LYS:HB3   | 2:b:5390:TYR:CE1   | 2.54                     | 0.42              |
| 22:b:6012:CLA:HAA1 | 22:b:6012:CLA:CBD  | 2.49                     | 0.42              |
| 3:c:5089:ILE:O     | 3:c:5111:PHE:HE2   | 2.00                     | 0.42              |
| 3:c:5397:THR:O     | 3:c:5399:ALA:N     | 2.52                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:c:6027:CLA:H3A  | 22:c:6027:CLA:CGA  | 2.50                     | 0.42              |
| 22:c:6029:CLA:HMA3 | 22:c:6029:CLA:HAA2 | 1.58                     | 0.42              |
| 5:e:5034:GLY:CA    | 6:f:5032:PHE:CD1   | 3.03                     | 0.42              |
| 6:f:5022:ALA:O     | 6:f:5023:VAL:C     | 2.62                     | 0.42              |
| 6:f:5034:LEU:HD13  | 9:j:5028:PHE:HZ    | 1.85                     | 0.42              |
| 25:k:6051:BCR:H371 | 25:k:6051:BCR:H24C | 1.64                     | 0.42              |
| 11:l:5024:ILE:HD11 | 12:m:5018:PRO:HB2  | 2.01                     | 0.42              |
| 18:y:5030:ILE:O    | 18:y:5030:ILE:CG1  | 2.67                     | 0.42              |
| 1:A:27:ARG:NH1     | 1:A:28:LEU:HD12    | 2.34                     | 0.42              |
| 1:A:41:LEU:HD22    | 1:A:41:LEU:H       | 1.83                     | 0.42              |
| 1:A:180:PHE:O      | 1:A:184:ILE:CD1    | 2.68                     | 0.42              |
| 2:B:65:PHE:CE1     | 22:B:1012:CLA:HED2 | 2.54                     | 0.42              |
| 2:B:230:ARG:O      | 2:B:231:MET:C      | 2.63                     | 0.42              |
| 2:B:311:PHE:HD2    | 2:B:311:PHE:O      | 2.03                     | 0.42              |
| 2:B:370:LEU:N      | 2:B:370:LEU:HD12   | 2.35                     | 0.42              |
| 22:B:1011:CLA:H2   | 22:B:1013:CLA:H91  | 1.93                     | 0.42              |
| 22:B:1011:CLA:ND   | 22:B:1013:CLA:H51  | 2.35                     | 0.42              |
| 3:C:62:PHE:HZ      | 10:K:28:ILE:HB     | 1.83                     | 0.42              |
| 3:C:166:ILE:CD1    | 3:C:248:GLY:HA3    | 2.44                     | 0.42              |
| 4:D:93:TRP:HA      | 4:D:99:GLY:H       | 1.84                     | 0.42              |
| 5:E:18:ARG:HG2     | 5:E:22:ILE:HD11    | 2.01                     | 0.42              |
| 5:E:27:ILE:CD1     | 5:E:27:ILE:N       | 2.82                     | 0.42              |
| 9:J:18:GLY:HA3     | 25:K:1051:BCR:H371 | 2.00                     | 0.42              |
| 13:O:37:VAL:O      | 13:O:37:VAL:HG13   | 2.19                     | 0.42              |
| 13:O:80:GLU:O      | 13:O:82:PRO:N      | 2.53                     | 0.42              |
| 13:O:134:VAL:HG23  | 13:O:142:ILE:HG22  | 2.02                     | 0.42              |
| 15:U:64:ILE:H      | 15:U:67:LEU:HD12   | 1.84                     | 0.42              |
| 1:a:5027:ARG:NH1   | 1:a:5028:LEU:HD12  | 2.34                     | 0.42              |
| 1:a:5063:ILE:HG12  | 1:a:5065:GLU:N     | 2.34                     | 0.42              |
| 1:a:5093:PHE:C     | 1:a:5095:PRO:HD3   | 2.45                     | 0.42              |
| 1:a:5104:GLU:CD    | 13:o:5099:ARG:HB3  | 2.44                     | 0.42              |
| 1:a:5105:TRP:CD1   | 1:a:5110:GLY:HA3   | 2.55                     | 0.42              |
| 1:a:5114:LEU:C     | 1:a:5114:LEU:HD12  | 2.44                     | 0.42              |
| 1:a:5121:LEU:O     | 1:a:5124:SER:N     | 2.51                     | 0.42              |
| 1:a:5206:PHE:CE2   | 22:d:6004:CLA:O1A  | 2.73                     | 0.42              |
| 1:a:5279:ARG:HD3   | 4:d:5208:ALA:C     | 2.45                     | 0.42              |
| 26:a:6063:LHG:C32  | 22:k:6034:CLA:C15  | 2.87                     | 0.42              |
| 2:b:5024:LEU:HA    | 22:b:6023:CLA:HED3 | 2.01                     | 0.42              |
| 2:b:5065:PHE:C     | 2:b:5067:ALA:H     | 2.28                     | 0.42              |
| 2:b:5065:PHE:CE1   | 22:b:6012:CLA:HED2 | 2.54                     | 0.42              |
| 2:b:5135:LEU:N     | 2:b:5135:LEU:CD1   | 2.80                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5139:PHE:CZ    | 22:h:6017:CLA:CMB  | 3.02                     | 0.42              |
| 2:b:5248:ALA:CA    | 22:b:6011:CLA:H51  | 2.50                     | 0.42              |
| 2:b:5332:LYS:O     | 2:b:5444:ARG:NH1   | 2.53                     | 0.42              |
| 2:b:5346:PHE:CD2   | 2:b:5346:PHE:N     | 2.87                     | 0.42              |
| 2:b:5447:PRO:O     | 2:b:5448:ARG:C     | 2.61                     | 0.42              |
| 22:b:6021:CLA:C12  | 28:b:6060:MGE:H132 | 2.50                     | 0.42              |
| 3:c:5042:LEU:HD23  | 3:c:5048:LYS:HG2   | 1.94                     | 0.42              |
| 3:c:5163:PHE:O     | 3:c:5166:ILE:HG12  | 2.19                     | 0.42              |
| 3:c:5296:VAL:HG23  | 3:c:5297:TYR:CE1   | 2.51                     | 0.42              |
| 3:c:5321:ASP:OD2   | 3:c:5321:ASP:N     | 2.52                     | 0.42              |
| 3:c:5377:LEU:O     | 3:c:5381:LYS:HB2   | 2.19                     | 0.42              |
| 22:c:6032:CLA:CAB  | 22:k:6034:CLA:CMC  | 2.53                     | 0.42              |
| 4:d:5069:GLU:HB3   | 5:e:5055:TYR:OH    | 2.19                     | 0.42              |
| 4:d:5199:MET:HG2   | 24:d:6042:PQ9:H352 | 2.02                     | 0.42              |
| 4:d:5238:THR:HG22  | 4:d:5239:GLN:HG2   | 2.01                     | 0.42              |
| 22:d:6005:CLA:HMA2 | 24:d:6042:PQ9:H443 | 2.01                     | 0.42              |
| 6:f:5015:ILE:HD12  | 31:f:6040:HEM:HMD1 | 2.02                     | 0.42              |
| 11:l:5036:PHE:CD1  | 12:m:5007:GLY:HA3  | 2.55                     | 0.42              |
| 13:o:5045:CYS:N    | 13:o:5072:GLN:NE2  | 2.61                     | 0.42              |
| 13:o:5059:ASP:CG   | 13:o:5061:SER:HB2  | 2.43                     | 0.42              |
| 13:o:5195:ASP:OD1  | 13:o:5195:ASP:C    | 2.62                     | 0.42              |
| 15:u:5009:LEU:H    | 15:u:5009:LEU:HG   | 1.47                     | 0.42              |
| 15:u:5026:ASP:HB3  | 15:u:5030:THR:H    | 1.84                     | 0.42              |
| 20:z:5045:GLY:O    | 20:z:5049:ALA:CB   | 2.67                     | 0.42              |
| 1:A:105:TRP:CH2    | 1:A:111:PRO:HA     | 2.55                     | 0.42              |
| 1:A:271:LEU:O      | 1:A:275:LEU:HG     | 2.19                     | 0.42              |
| 1:A:285:PHE:O      | 1:A:289:GLY:N      | 2.49                     | 0.42              |
| 2:B:21:ALA:HB2     | 2:B:114:HIS:HB2    | 2.02                     | 0.42              |
| 2:B:248:ALA:CA     | 22:B:1011:CLA:H51  | 2.50                     | 0.42              |
| 2:B:392:PHE:HE2    | 2:B:417:VAL:HG12   | 1.85                     | 0.42              |
| 3:C:64:ALA:O       | 3:C:68:THR:CB      | 2.68                     | 0.42              |
| 3:C:119:LEU:HD11   | 25:C:1052:BCR:C34  | 2.48                     | 0.42              |
| 3:C:377:LEU:C      | 3:C:377:LEU:CD1    | 2.92                     | 0.42              |
| 22:C:1037:CLA:H121 | 22:C:1037:CLA:H162 | 1.26                     | 0.42              |
| 7:H:28:THR:N       | 22:H:1017:CLA:OBD  | 2.52                     | 0.42              |
| 8:I:14:PHE:CE1     | 8:I:18:LEU:HD12    | 2.43                     | 0.42              |
| 11:L:24:ILE:HD11   | 12:M:18:PRO:HB2    | 2.01                     | 0.42              |
| 12:M:32:GLN:HE21   | 12:M:32:GLN:CA     | 2.25                     | 0.42              |
| 13:O:104:LEU:CD1   | 13:O:107:ILE:HD11  | 2.49                     | 0.42              |
| 13:O:234:THR:HB    | 13:O:236:GLU:HG3   | 2.01                     | 0.42              |
| 15:U:11:ASN:OD1    | 15:U:11:ASN:C      | 2.63                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5038:ILE:HB    | 1:a:5039:PRO:HD3   | 2.02                     | 0.42              |
| 2:b:5006:TYR:OH    | 28:b:6060:MGE:H3D  | 2.19                     | 0.42              |
| 2:b:5021:ALA:HB2   | 2:b:5114:HIS:HB2   | 2.02                     | 0.42              |
| 2:b:5150:CYS:N     | 22:b:6011:CLA:HBC2 | 2.33                     | 0.42              |
| 2:b:5359:MET:HA    | 2:b:5360:PRO:HD2   | 1.85                     | 0.42              |
| 2:b:5429:ILE:HG22  | 2:b:5430:PHE:N     | 2.34                     | 0.42              |
| 22:b:6010:CLA:C3D  | 22:b:6011:CLA:CMB  | 2.98                     | 0.42              |
| 28:b:6060:MGE:H5B2 | 4:d:5276:VAL:CG2   | 2.50                     | 0.42              |
| 3:c:5054:VAL:HG12  | 3:c:5125:LEU:O     | 2.19                     | 0.42              |
| 3:c:5062:PHE:CE2   | 10:k:5029:PRO:HG3  | 2.55                     | 0.42              |
| 3:c:5171:GLY:HA2   | 3:c:5174:LEU:H     | 1.85                     | 0.42              |
| 3:c:5332:GLN:NE2   | 13:o:5175:PRO:HG3  | 2.34                     | 0.42              |
| 4:d:5161:PRO:HG3   | 4:d:5170:ALA:HA    | 2.02                     | 0.42              |
| 4:d:5166:SER:C     | 4:d:5168:PHE:N     | 2.75                     | 0.42              |
| 28:d:6062:MGE:H1D  | 28:d:6062:MGE:H2G  | 1.40                     | 0.42              |
| 22:k:6034:CLA:CGA  | 22:k:6034:CLA:C1A  | 2.97                     | 0.42              |
| 13:o:5134:VAL:HG23 | 13:o:5142:ILE:HG22 | 2.02                     | 0.42              |
| 15:u:5036:ILE:HG22 | 15:u:5042:TYR:HB2  | 2.02                     | 0.42              |
| 18:y:5021:GLN:O    | 18:y:5025:ILE:CG2  | 2.65                     | 0.42              |
| 1:A:37:MET:SD      | 1:A:126:TYR:CB     | 3.08                     | 0.42              |
| 1:A:104:GLU:CD     | 13:O:99:ARG:HB3    | 2.44                     | 0.42              |
| 1:A:161:TYR:N      | 1:A:162:PRO:CD     | 2.83                     | 0.42              |
| 1:A:206:PHE:CE2    | 22:D:1004:CLA:O1A  | 2.73                     | 0.42              |
| 1:A:304:HIS:HE1    | 16:V:163:TYR:O     | 2.03                     | 0.42              |
| 1:A:328:MET:HE1    | 4:D:183:LEU:HD13   | 2.02                     | 0.42              |
| 22:A:1006:CLA:HAA1 | 22:A:1006:CLA:CBD  | 2.49                     | 0.42              |
| 23:A:1038:PHO:OBD  | 23:A:1038:PHO:O2D  | 2.38                     | 0.42              |
| 26:A:1063:LHG:HC11 | 3:C:447:ARG:HH12   | 1.85                     | 0.42              |
| 2:B:188:ASP:CB     | 7:H:58:VAL:HG22    | 2.50                     | 0.42              |
| 2:B:313:ASP:OD2    | 2:B:358:ARG:NH2    | 2.50                     | 0.42              |
| 2:B:326:ARG:NH2    | 2:B:442:ILE:CG2    | 2.83                     | 0.42              |
| 3:C:45:LEU:HA      | 3:C:45:LEU:HD23    | 1.75                     | 0.42              |
| 3:C:146:PHE:O      | 3:C:147:PHE:HB2    | 2.19                     | 0.42              |
| 3:C:342:MET:HG2    | 3:C:343:ARG:N      | 2.34                     | 0.42              |
| 4:D:186:GLN:CD     | 4:D:322:ASN:HD21   | 2.28                     | 0.42              |
| 5:E:48:GLY:O       | 5:E:49:THR:C       | 2.61                     | 0.42              |
| 5:E:74:GLN:O       | 5:E:77:GLU:HB2     | 2.20                     | 0.42              |
| 7:H:28:THR:O       | 7:H:31:MET:N       | 2.44                     | 0.42              |
| 12:M:8:PHE:O       | 12:M:12:ALA:CB     | 2.67                     | 0.42              |
| 14:T:28:ARG:HA     | 14:T:28:ARG:HE     | 1.83                     | 0.42              |
| 15:U:26:ASP:HB3    | 15:U:30:THR:H      | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:V:47:LEU:CG     | 16:V:48:THR:H      | 2.33                     | 0.42              |
| 16:V:105:PRO:HG2   | 16:V:115:ALA:HA    | 2.00                     | 0.42              |
| 18:Y:30:ILE:O      | 18:Y:30:ILE:HG12   | 2.20                     | 0.42              |
| 18:Y:43:ARG:CD     | 20:Z:31:GLN:HE21   | 2.28                     | 0.42              |
| 1:a:5078:ILE:HD13  | 11:l:5033:SER:CB   | 2.50                     | 0.42              |
| 1:a:5096:ILE:O     | 1:a:5096:ILE:HG22  | 2.20                     | 0.42              |
| 1:a:5140:ARG:HB2   | 4:d:5220:ASN:HA    | 2.01                     | 0.42              |
| 1:a:5244:GLU:HA    | 4:d:5264:LYS:HZ1   | 1.84                     | 0.42              |
| 1:a:5280:VAL:CG2   | 4:d:5212:ALA:HB1   | 2.49                     | 0.42              |
| 1:a:5285:PHE:O     | 1:a:5289:GLY:N     | 2.49                     | 0.42              |
| 2:b:5188:ASP:CB    | 7:h:5058:VAL:HG22  | 2.50                     | 0.42              |
| 2:b:5314:TYR:O     | 2:b:5315:ILE:C     | 2.62                     | 0.42              |
| 2:b:5486:LEU:O     | 2:b:5487:SER:HB2   | 2.18                     | 0.42              |
| 22:b:6016:CLA:HAA1 | 22:b:6016:CLA:CBD  | 2.49                     | 0.42              |
| 22:b:6023:CLA:H92  | 22:b:6023:CLA:H62  | 1.85                     | 0.42              |
| 3:c:5046:SER:O     | 3:c:5047:GLY:C     | 2.59                     | 0.42              |
| 3:c:5422:PRO:O     | 3:c:5426:LEU:HD13  | 2.20                     | 0.42              |
| 22:c:6026:CLA:C3   | 22:c:6026:CLA:CGA  | 2.96                     | 0.42              |
| 4:d:5111:TRP:C     | 4:d:5113:PHE:N     | 2.77                     | 0.42              |
| 4:d:5186:GLN:CD    | 4:d:5322:ASN:HD21  | 2.28                     | 0.42              |
| 12:m:5009:ILE:HD12 | 12:m:5009:ILE:N    | 2.32                     | 0.42              |
| 12:m:5028:GLN:CD   | 12:m:5028:GLN:C    | 2.88                     | 0.42              |
| 13:o:5036:ILE:O    | 13:o:5036:ILE:CG2  | 2.66                     | 0.42              |
| 16:v:5131:ARG:C    | 16:v:5133:LEU:H    | 2.27                     | 0.42              |
| 20:z:5044:SER:O    | 20:z:5048:ILE:CD1  | 2.66                     | 0.42              |
| 1:A:38:ILE:CB      | 1:A:39:PRO:HD3     | 2.50                     | 0.42              |
| 1:A:129:ARG:NH1    | 4:D:256:ILE:HD12   | 2.32                     | 0.42              |
| 1:A:131:TRP:CE3    | 1:A:132:GLU:N      | 2.87                     | 0.42              |
| 1:A:142:TRP:HE1    | 4:D:219:GLU:HB3    | 1.84                     | 0.42              |
| 22:A:1003:CLA:HAB  | 22:D:1004:CLA:C4B  | 2.49                     | 0.42              |
| 23:A:1038:PHO:H91  | 22:D:1005:CLA:C17  | 2.49                     | 0.42              |
| 2:B:49:ASP:HA      | 13:o:5083:LYS:HE3  | 2.01                     | 0.42              |
| 2:B:150:CYS:N      | 22:B:1011:CLA:HBC2 | 2.34                     | 0.42              |
| 2:B:228:ALA:C      | 2:B:230:ARG:H      | 2.27                     | 0.42              |
| 2:B:307:GLU:OE2    | 13:o:5085:LYS:CB   | 2.64                     | 0.42              |
| 2:B:486:LEU:O      | 2:B:487:SER:HB2    | 2.19                     | 0.42              |
| 22:B:1010:CLA:H61  | 22:B:1010:CLA:H41  | 1.84                     | 0.42              |
| 22:B:1020:CLA:HMC1 | 22:B:1020:CLA:HBC2 | 2.02                     | 0.42              |
| 3:C:130:VAL:O      | 3:C:134:ILE:CD1    | 2.68                     | 0.42              |
| 3:C:157:MET:HE2    | 3:C:271:TYR:CE2    | 2.55                     | 0.42              |
| 3:C:466:VAL:C      | 3:C:468:SER:N      | 2.77                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:C:1033:CLA:H202 | 22:C:1033:CLA:H162 | 1.78                     | 0.42              |
| 10:K:35:LEU:O      | 10:K:37:PHE:N      | 2.53                     | 0.42              |
| 12:M:18:PRO:CG     | 12:M:19:SER:N      | 2.83                     | 0.42              |
| 15:U:28:ASN:ND2    | 15:U:54:PRO:HB2    | 2.24                     | 0.42              |
| 17:X:13:THR:O      | 17:X:15:SER:N      | 2.53                     | 0.42              |
| 20:Z:5:PHE:O       | 20:Z:8:ALA:HB3     | 2.19                     | 0.42              |
| 1:a:5020:TRP:O     | 1:a:5021:VAL:C     | 2.59                     | 0.42              |
| 1:a:5103:ASP:HA    | 1:a:5106:LEU:CD1   | 2.39                     | 0.42              |
| 1:a:5185:VAL:HG12  | 1:a:5186:PHE:N     | 2.34                     | 0.42              |
| 1:a:5271:LEU:O     | 1:a:5275:LEU:HG    | 2.19                     | 0.42              |
| 1:a:5271:LEU:CG    | 1:a:5272:HIS:N     | 2.83                     | 0.42              |
| 1:a:5340:PRO:CD    | 15:u:5103:TYR:CE2  | 3.03                     | 0.42              |
| 2:b:5172:TYR:CD2   | 2:b:5173:GLY:N     | 2.88                     | 0.42              |
| 2:b:5247:PHE:O     | 2:b:5247:PHE:CD1   | 2.72                     | 0.42              |
| 2:b:5385:ARG:HE    | 2:b:5385:ARG:HB2   | 1.14                     | 0.42              |
| 2:b:5472:ARG:CD    | 22:b:6019:CLA:HED3 | 2.50                     | 0.42              |
| 22:b:6011:CLA:ND   | 22:b:6013:CLA:H51  | 2.35                     | 0.42              |
| 22:b:6012:CLA:C2C  | 22:b:6021:CLA:CBB  | 2.98                     | 0.42              |
| 22:b:6012:CLA:H61  | 22:b:6012:CLA:H41  | 1.88                     | 0.42              |
| 3:c:5187:ASP:C     | 3:c:5187:ASP:OD2   | 2.62                     | 0.42              |
| 3:c:5451:ALA:HA    | 3:c:5456:GLU:CG    | 2.48                     | 0.42              |
| 22:c:6029:CLA:H92  | 22:c:6029:CLA:H62  | 1.80                     | 0.42              |
| 4:d:5120:PHE:CD1   | 4:d:5123:ILE:HD12  | 2.55                     | 0.42              |
| 5:e:5022:ILE:O     | 5:e:5025:ILE:HG13  | 2.18                     | 0.42              |
| 12:m:5018:PRO:CG   | 12:m:5019:SER:N    | 2.83                     | 0.42              |
| 13:o:5156:GLN:HA   | 13:o:5157:PRO:HD3  | 1.86                     | 0.42              |
| 13:o:5162:ILE:HD13 | 13:o:5269:ILE:HD12 | 2.01                     | 0.42              |
| 13:o:5180:ALA:HB2  | 15:u:5090:ALA:O    | 2.20                     | 0.42              |
| 13:o:5254:HIS:H    | 13:o:5254:HIS:CD2  | 2.38                     | 0.42              |
| 15:u:5078:ASN:C    | 15:u:5080:GLU:N    | 2.78                     | 0.42              |
| 16:v:5035:THR:HG23 | 16:v:5046:THR:H    | 1.85                     | 0.42              |
| 16:v:5101:TYR:CE2  | 31:v:6041:HEM:HAA1 | 2.54                     | 0.42              |
| 16:v:5106:THR:HA   | 16:v:5114:ILE:HG22 | 2.00                     | 0.42              |
| 1:A:37:MET:SD      | 1:A:126:TYR:HA     | 2.59                     | 0.42              |
| 1:A:81:ALA:CA      | 1:A:175:GLY:HA3    | 2.49                     | 0.42              |
| 1:A:99:ALA:O       | 1:A:100:ALA:O      | 2.38                     | 0.42              |
| 1:A:134:SER:HA     | 1:A:139:MET:HG2    | 2.01                     | 0.42              |
| 1:A:147:TYR:CA     | 23:A:1038:PHO:HMD2 | 2.50                     | 0.42              |
| 1:A:262:TYR:C      | 1:A:264:SER:H      | 2.27                     | 0.42              |
| 1:A:310:LYS:HG2    | 16:V:151:ILE:CG2   | 2.46                     | 0.42              |
| 1:A:318:ALA:HA     | 1:A:321:ILE:CD1    | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:330:VAL:HG21   | 4:D:328:TRP:CZ2    | 2.55                     | 0.42              |
| 2:B:49:ASP:HA      | 2:B:50:PRO:HD3     | 1.86                     | 0.42              |
| 2:B:99:ALA:O       | 2:B:101:ILE:N      | 2.53                     | 0.42              |
| 2:B:215:PHE:CE2    | 2:B:219:VAL:HG21   | 2.55                     | 0.42              |
| 2:B:463:PHE:CD2    | 29:B:1058:DGD:HAV1 | 2.54                     | 0.42              |
| 22:B:1011:CLA:CAD  | 22:B:1013:CLA:H11  | 2.48                     | 0.42              |
| 22:B:1015:CLA:HAA1 | 22:B:1015:CLA:CBD  | 2.50                     | 0.42              |
| 3:C:276:LEU:HD22   | 3:C:441:HIS:N      | 2.34                     | 0.42              |
| 22:C:1032:CLA:H18  | 29:C:1056:DGD:HBH1 | 2.02                     | 0.42              |
| 4:D:69:GLU:HB3     | 5:E:55:TYR:OH      | 2.19                     | 0.42              |
| 4:D:87:HIS:O       | 4:D:88:SER:C       | 2.63                     | 0.42              |
| 4:D:97:ALA:HB1     | 4:D:104:TRP:HB2    | 2.02                     | 0.42              |
| 4:D:238:THR:HG22   | 4:D:239:GLN:HG2    | 2.01                     | 0.42              |
| 7:H:41:PHE:CD1     | 25:H:1049:BCR:H362 | 2.49                     | 0.42              |
| 11:L:19:LEU:O      | 11:L:20:GLY:C      | 2.61                     | 0.42              |
| 11:L:24:ILE:C      | 11:L:26:VAL:N      | 2.76                     | 0.42              |
| 13:O:76:PHE:CD1    | 13:O:261:ILE:HD12  | 2.54                     | 0.42              |
| 16:V:81:ARG:O      | 16:V:82:THR:C      | 2.62                     | 0.42              |
| 16:V:94:ASN:O      | 16:V:95:ILE:C      | 2.63                     | 0.42              |
| 16:V:156:TRP:HA    | 16:V:156:TRP:CE3   | 2.55                     | 0.42              |
| 18:Y:35:ILE:CD1    | 18:Y:36:ILE:HD12   | 2.50                     | 0.42              |
| 1:a:5047:CYS:HA    | 25:a:6044:BCR:H372 | 2.02                     | 0.42              |
| 1:a:5219:VAL:HG21  | 4:d:5268:HIS:CG    | 2.54                     | 0.42              |
| 1:a:5295:PHE:HD2   | 3:c:5291:TRP:CE2   | 2.37                     | 0.42              |
| 1:a:5309:ALA:HB3   | 16:v:5028:GLU:CB   | 2.47                     | 0.42              |
| 1:a:5310:LYS:N     | 16:v:5028:GLU:HB2  | 2.34                     | 0.42              |
| 1:a:5330:VAL:HG21  | 4:d:5328:TRP:CZ2   | 2.55                     | 0.42              |
| 2:b:5013:ILE:HD12  | 2:b:5234:ILE:HG23  | 2.01                     | 0.42              |
| 2:b:5067:ALA:CB    | 2:b:5267:LEU:HD21  | 2.50                     | 0.42              |
| 2:b:5115:TRP:O     | 2:b:5116:VAL:C     | 2.63                     | 0.42              |
| 2:b:5188:ASP:OD1   | 7:h:5058:VAL:HA    | 2.19                     | 0.42              |
| 2:b:5246:PHE:HB3   | 2:b:5462:PHE:HB3   | 2.01                     | 0.42              |
| 2:b:5297:THR:O     | 2:b:5298:LEU:C     | 2.60                     | 0.42              |
| 22:b:6022:CLA:OBD  | 11:l:5010:VAL:HG21 | 2.20                     | 0.42              |
| 3:c:5376:ASP:OD1   | 3:c:5379:LYS:HG3   | 2.20                     | 0.42              |
| 22:c:6025:CLA:CMB  | 25:c:6054:BCR:C24  | 2.98                     | 0.42              |
| 29:c:6057:DGD:HAS2 | 28:d:6059:MGE:CDB  | 2.47                     | 0.42              |
| 4:d:5027:PHE:HD1   | 6:f:5019:ARG:HG3   | 1.85                     | 0.42              |
| 4:d:5054:PHE:CD1   | 5:e:5047:PHE:HE1   | 2.38                     | 0.42              |
| 4:d:5249:ALA:O     | 4:d:5252:PHE:N     | 2.41                     | 0.42              |
| 4:d:5321:LEU:O     | 4:d:5322:ASN:C     | 2.63                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:d:6004:CLA:HHC  | 22:d:6004:CLA:CBB  | 2.21                     | 0.42              |
| 5:e:5077:GLU:O     | 5:e:5080:LEU:N     | 2.53                     | 0.42              |
| 11:l:5019:LEU:O    | 11:l:5020:GLY:C    | 2.61                     | 0.42              |
| 13:o:5052:ALA:CB   | 13:o:5229:LYS:HA   | 2.50                     | 0.42              |
| 13:o:5080:GLU:O    | 13:o:5082:PRO:N    | 2.53                     | 0.42              |
| 13:o:5187:GLY:O    | 13:o:5194:TYR:N    | 2.51                     | 0.42              |
| 16:v:5094:ASN:O    | 16:v:5095:ILE:C    | 2.63                     | 0.42              |
| 16:v:5107:THR:C    | 16:v:5109:ASP:H    | 2.26                     | 0.42              |
| 18:y:5030:ILE:O    | 18:y:5030:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:114:LEU:C      | 1:A:114:LEU:HD12   | 2.44                     | 0.41              |
| 1:A:193:LEU:O      | 1:A:193:LEU:CD2    | 2.68                     | 0.41              |
| 1:A:252:HIS:ND1    | 1:A:266:ASN:HB3    | 2.35                     | 0.41              |
| 1:A:310:LYS:N      | 16:V:28:GLU:HB2    | 2.34                     | 0.41              |
| 1:A:340:PRO:CD     | 15:U:103:TYR:CE2   | 3.03                     | 0.41              |
| 2:B:24:LEU:CG      | 2:B:111:ALA:HA     | 2.50                     | 0.41              |
| 2:B:65:PHE:C       | 2:B:67:ALA:H       | 2.28                     | 0.41              |
| 2:B:238:LEU:N      | 22:B:1020:CLA:CMD  | 2.82                     | 0.41              |
| 2:B:394:GLN:HB3    | 15:U:17:LEU:HD22   | 2.01                     | 0.41              |
| 22:B:1016:CLA:C16  | 22:D:1008:CLA:HMA3 | 2.38                     | 0.41              |
| 22:B:1016:CLA:C19  | 22:H:1017:CLA:H191 | 2.16                     | 0.41              |
| 3:C:79:LYS:O       | 3:C:84:GLN:NE2     | 2.53                     | 0.41              |
| 3:C:154:LYS:HE3    | 3:C:261:ARG:HE     | 1.83                     | 0.41              |
| 3:C:224:ILE:HG22   | 3:C:289:PHE:CE1    | 2.55                     | 0.41              |
| 3:C:425:TRP:CD1    | 22:C:1028:CLA:HMA2 | 2.55                     | 0.41              |
| 3:C:451:ALA:O      | 3:C:454:GLY:N      | 2.53                     | 0.41              |
| 4:D:54:PHE:CD1     | 5:E:47:PHE:HE1     | 2.38                     | 0.41              |
| 4:D:111:TRP:C      | 4:D:113:PHE:N      | 2.77                     | 0.41              |
| 4:D:197:HIS:ND1    | 4:D:197:HIS:C      | 2.76                     | 0.41              |
| 4:D:267:LEU:C      | 4:D:269:PHE:N      | 2.78                     | 0.41              |
| 5:E:34:GLY:O       | 5:E:37:PHE:HB3     | 2.20                     | 0.41              |
| 10:K:17:ILE:H      | 10:K:17:ILE:HG13   | 1.47                     | 0.41              |
| 25:K:1051:BCR:H371 | 25:K:1051:BCR:H24C | 1.64                     | 0.41              |
| 12:M:31:SER:O      | 12:m:5032:GLN:NE2  | 2.53                     | 0.41              |
| 13:O:156:GLN:HA    | 13:O:157:PRO:HD3   | 1.86                     | 0.41              |
| 13:O:175:PRO:HG2   | 13:O:176:SER:N     | 2.34                     | 0.41              |
| 13:O:180:ALA:HB2   | 15:U:90:ALA:O      | 2.20                     | 0.41              |
| 13:O:192:SER:OG    | 13:O:193:GLY:N     | 2.53                     | 0.41              |
| 15:U:45:LEU:HD12   | 15:U:45:LEU:HA     | 1.95                     | 0.41              |
| 16:V:32:GLU:C      | 16:V:34:LEU:N      | 2.76                     | 0.41              |
| 16:V:148:GLU:O     | 16:V:151:ILE:CD1   | 2.68                     | 0.41              |
| 20:Z:33:TRP:O      | 20:Z:37:LYS:HB3    | 2.19                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5060:ILE:O     | 1:a:5061:ASP:C     | 2.63                     | 0.41              |
| 1:a:5137:LEU:HB3   | 1:a:5139:MET:HE3   | 2.00                     | 0.41              |
| 1:a:5328:MET:HE1   | 4:d:5183:LEU:HD13  | 2.02                     | 0.41              |
| 26:a:6063:LHG:O9   | 26:a:6063:LHG:C6   | 2.52                     | 0.41              |
| 2:b:5020:ILE:O     | 2:b:5024:LEU:CB    | 2.68                     | 0.41              |
| 2:b:5056:TRP:HZ3   | 2:b:5317:ASN:OD1   | 2.03                     | 0.41              |
| 2:b:5215:PHE:CE2   | 2:b:5219:VAL:HG21  | 2.55                     | 0.41              |
| 2:b:5460:LEU:O     | 4:d:5280:TRP:CZ3   | 2.70                     | 0.41              |
| 22:b:6020:CLA:HMC1 | 22:b:6020:CLA:HBC2 | 2.02                     | 0.41              |
| 22:b:6022:CLA:CGD  | 22:b:6022:CLA:CAA  | 2.65                     | 0.41              |
| 3:c:5056:HIS:HD2   | 3:c:5057:ALA:CA    | 2.33                     | 0.41              |
| 3:c:5130:VAL:O     | 3:c:5134:ILE:CD1   | 2.68                     | 0.41              |
| 3:c:5168:LEU:HB3   | 22:c:6025:CLA:HMC2 | 2.02                     | 0.41              |
| 3:c:5367:GLU:O     | 3:c:5368:PRO:C     | 2.61                     | 0.41              |
| 3:c:5435:PHE:O     | 3:c:5436:PHE:C     | 2.63                     | 0.41              |
| 3:c:5461:ARG:HE    | 4:d:5223:PHE:HD2   | 1.64                     | 0.41              |
| 29:c:6056:DGD:HB61 | 29:c:6056:DGD:HB91 | 1.80                     | 0.41              |
| 4:d:5053:THR:HG22  | 4:d:5067:TYR:HD2   | 1.85                     | 0.41              |
| 4:d:5145:ALA:HB2   | 4:d:5272:LEU:HD12  | 2.00                     | 0.41              |
| 25:d:6050:BCR:C16  | 25:d:6050:BCR:H351 | 2.48                     | 0.41              |
| 5:e:5013:ILE:HG13  | 5:e:5013:ILE:O     | 2.18                     | 0.41              |
| 6:f:5043:ILE:HG13  | 6:f:5043:ILE:H     | 1.54                     | 0.41              |
| 7:h:5035:MET:O     | 7:h:5038:PHE:HB3   | 2.20                     | 0.41              |
| 13:o:5076:PHE:CD1  | 13:o:5261:ILE:HD12 | 2.54                     | 0.41              |
| 13:o:5092:VAL:CG1  | 13:o:5093:PRO:CD   | 2.97                     | 0.41              |
| 13:o:5105:ASP:OD1  | 13:o:5105:ASP:C    | 2.63                     | 0.41              |
| 15:u:5064:ILE:H    | 15:u:5067:LEU:HD12 | 1.84                     | 0.41              |
| 1:A:187:GLN:HG2    | 1:A:328:MET:HE1    | 2.02                     | 0.41              |
| 1:A:269:ARG:NE     | 4:D:222:LEU:HD21   | 2.35                     | 0.41              |
| 2:B:115:TRP:O      | 2:B:116:VAL:C      | 2.63                     | 0.41              |
| 2:B:158:LEU:C      | 2:B:160:GLY:N      | 2.78                     | 0.41              |
| 2:B:246:PHE:HB3    | 2:B:462:PHE:HB3    | 2.01                     | 0.41              |
| 2:B:385:ARG:HE     | 2:B:385:ARG:HB2    | 1.14                     | 0.41              |
| 2:B:424:ALA:C      | 2:B:426:PHE:N      | 2.77                     | 0.41              |
| 3:C:56:HIS:HD2     | 3:C:57:ALA:CA      | 2.33                     | 0.41              |
| 3:C:157:MET:HB3    | 22:C:1031:CLA:CBC  | 2.49                     | 0.41              |
| 3:C:165:LEU:HD21   | 22:C:1030:CLA:CBB  | 2.50                     | 0.41              |
| 3:C:171:GLY:HA2    | 3:C:174:LEU:H      | 1.85                     | 0.41              |
| 3:C:239:TRP:O      | 3:C:243:ILE:CG1    | 2.67                     | 0.41              |
| 3:C:309:ALA:O      | 3:C:311:GLN:N      | 2.53                     | 0.41              |
| 3:C:337:LEU:HA     | 3:C:337:LEU:HD23   | 1.80                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:343:ARG:NH2    | 13:O:103:SER:O     | 2.47                     | 0.41              |
| 3:C:348:GLU:CB     | 13:O:42:ALA:CB     | 2.84                     | 0.41              |
| 22:C:1035:CLA:H93  | 22:C:1035:CLA:H2   | 2.02                     | 0.41              |
| 4:D:21:TRP:CE3     | 4:D:22:LEU:HB3     | 2.55                     | 0.41              |
| 4:D:46:GLY:HA2     | 25:D:1050:BCR:H10C | 2.02                     | 0.41              |
| 4:D:122:LEU:HD22   | 4:D:122:LEU:N      | 2.34                     | 0.41              |
| 7:H:31:MET:SD      | 22:H:1017:CLA:CAA  | 3.04                     | 0.41              |
| 7:H:35:MET:O       | 7:H:38:PHE:HB3     | 2.20                     | 0.41              |
| 10:K:35:LEU:HD22   | 25:K:1051:BCR:H352 | 2.02                     | 0.41              |
| 13:O:231:ASP:CB    | 13:O:234:THR:OG1   | 2.65                     | 0.41              |
| 25:T:6046:BCR:H371 | 25:T:6046:BCR:H24C | 1.61                     | 0.41              |
| 25:T:6048:BCR:C30  | 25:T:6048:BCR:C37  | 2.61                     | 0.41              |
| 16:V:101:TYR:O     | 16:V:104:ASN:C     | 2.63                     | 0.41              |
| 16:V:128:PRO:O     | 16:V:129:LYS:C     | 2.63                     | 0.41              |
| 16:V:131:ARG:C     | 16:V:133:LEU:H     | 2.27                     | 0.41              |
| 16:V:156:TRP:HA    | 16:V:156:TRP:HE3   | 1.85                     | 0.41              |
| 1:a:5038:ILE:CB    | 1:a:5039:PRO:HD3   | 2.50                     | 0.41              |
| 1:a:5041:LEU:HD22  | 1:a:5041:LEU:H     | 1.83                     | 0.41              |
| 1:a:5258:LEU:C     | 1:a:5259:ILE:CG1   | 2.92                     | 0.41              |
| 1:a:5269:ARG:NE    | 4:d:5222:LEU:HD21  | 2.35                     | 0.41              |
| 1:a:5309:ALA:HB3   | 16:v:5028:GLU:CG   | 2.50                     | 0.41              |
| 1:a:5323:ARG:CG    | 4:d:5329:MET:HA    | 2.50                     | 0.41              |
| 22:a:6006:CLA:H162 | 22:a:6006:CLA:H192 | 1.79                     | 0.41              |
| 2:b:5041:GLU:HB3   | 2:b:5060:MET:SD    | 2.60                     | 0.41              |
| 2:b:5098:LEU:O     | 2:b:5102:VAL:HG22  | 2.20                     | 0.41              |
| 2:b:5235:GLU:CG    | 2:b:5473:THR:HA    | 2.49                     | 0.41              |
| 2:b:5373:LYS:H     | 2:b:5373:LYS:HG2   | 1.32                     | 0.41              |
| 2:b:5392:PHE:CE2   | 2:b:5418:LYS:HA    | 2.55                     | 0.41              |
| 22:b:6015:CLA:H161 | 22:b:6015:CLA:H141 | 1.77                     | 0.41              |
| 3:c:5157:MET:HB3   | 22:c:6031:CLA:CBC  | 2.50                     | 0.41              |
| 3:c:5160:ILE:C     | 3:c:5162:GLY:N     | 2.76                     | 0.41              |
| 3:c:5165:LEU:HD21  | 22:c:6030:CLA:CBB  | 2.50                     | 0.41              |
| 3:c:5239:TRP:O     | 3:c:5243:ILE:CG1   | 2.67                     | 0.41              |
| 3:c:5318:LEU:HD23  | 3:c:5318:LEU:C     | 2.45                     | 0.41              |
| 4:d:5282:SER:HB2   | 22:d:6004:CLA:HED3 | 2.01                     | 0.41              |
| 4:d:5315:TYR:CZ    | 4:d:5319:LEU:HD12  | 2.55                     | 0.41              |
| 22:d:6005:CLA:CMA  | 24:d:6042:PQ9:H443 | 2.50                     | 0.41              |
| 5:e:5034:GLY:O     | 5:e:5037:PHE:HB3   | 2.20                     | 0.41              |
| 6:f:5041:GLN:HG3   | 9:j:5027:LEU:HG    | 2.01                     | 0.41              |
| 13:o:5185:PRO:O    | 13:o:5186:LYS:CB   | 2.68                     | 0.41              |
| 15:u:5011:ASN:OD1  | 15:u:5011:ASN:C    | 2.63                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:v:5101:TYR:O    | 16:v:5102:MET:C    | 2.63                     | 0.41              |
| 16:v:5101:TYR:O    | 16:v:5104:ASN:C    | 2.63                     | 0.41              |
| 17:x:5013:THR:O    | 17:x:5015:SER:N    | 2.53                     | 0.41              |
| 1:A:215:HIS:HD2    | 1:A:275:LEU:CD1    | 2.33                     | 0.41              |
| 1:A:278:TRP:CE3    | 1:A:278:TRP:CA     | 2.94                     | 0.41              |
| 2:B:56:TRP:HZ3     | 2:B:317:ASN:OD1    | 2.03                     | 0.41              |
| 2:B:407:ASN:C      | 2:B:409:GLN:H      | 2.29                     | 0.41              |
| 2:B:445:THR:OG1    | 2:B:449:GLY:HA3    | 2.20                     | 0.41              |
| 22:B:1012:CLA:C2C  | 22:B:1021:CLA:CBB  | 2.98                     | 0.41              |
| 22:B:1021:CLA:HED2 | 22:B:1021:CLA:NA   | 2.20                     | 0.41              |
| 28:B:1060:MGE:H5B2 | 4:D:276:VAL:CG2    | 2.50                     | 0.41              |
| 3:C:274:TYR:CE2    | 22:C:1031:CLA:HMC1 | 2.54                     | 0.41              |
| 22:C:1025:CLA:CMB  | 25:C:1054:BCR:C24  | 2.98                     | 0.41              |
| 22:C:1026:CLA:HAA1 | 22:C:1026:CLA:CBD  | 2.50                     | 0.41              |
| 22:C:1028:CLA:H161 | 22:C:1028:CLA:H202 | 1.61                     | 0.41              |
| 4:D:236:ASN:OD1    | 4:D:239:GLN:O      | 2.37                     | 0.41              |
| 4:D:292:ASN:O      | 4:D:294:ARG:HG2    | 2.20                     | 0.41              |
| 4:D:346:LEU:HA     | 4:D:347:PRO:HD2    | 1.86                     | 0.41              |
| 24:D:1042:PQ9:H201 | 24:D:1042:PQ9:H162 | 1.84                     | 0.41              |
| 7:H:27:THR:C       | 22:H:1017:CLA:OBD  | 2.63                     | 0.41              |
| 7:H:40:VAL:HG12    | 7:H:44:ILE:HG12    | 2.03                     | 0.41              |
| 8:I:3:THR:O        | 8:I:6:ILE:HG13     | 2.20                     | 0.41              |
| 12:M:20:VAL:O      | 12:M:24:ILE:HG13   | 2.20                     | 0.41              |
| 12:M:28:GLN:CD     | 12:M:28:GLN:C      | 2.88                     | 0.41              |
| 13:O:105:ASP:OD1   | 13:O:105:ASP:C     | 2.63                     | 0.41              |
| 25:T:6046:BCR:C35  | 25:b:6047:BCR:H23C | 2.50                     | 0.41              |
| 15:U:78:ASN:C      | 15:U:80:GLU:N      | 2.78                     | 0.41              |
| 18:Y:43:ARG:CZ     | 20:Z:29:SER:HB3    | 2.49                     | 0.41              |
| 1:a:5062:GLY:CA    | 1:a:5087:ASN:HB2   | 2.46                     | 0.41              |
| 1:a:5134:SER:HA    | 1:a:5139:MET:HG2   | 2.01                     | 0.41              |
| 1:a:5135:TYR:HE1   | 3:c:5449:ARG:O     | 2.03                     | 0.41              |
| 24:a:6043:PQ9:H451 | 28:d:6059:MGE:CBA  | 2.49                     | 0.41              |
| 2:b:5006:TYR:H     | 2:b:5006:TYR:HD2   | 1.57                     | 0.41              |
| 2:b:5158:LEU:C     | 2:b:5160:GLY:H     | 2.28                     | 0.41              |
| 2:b:5158:LEU:C     | 2:b:5160:GLY:N     | 2.78                     | 0.41              |
| 2:b:5191:ASN:HD21  | 7:h:5060:VAL:CA    | 2.19                     | 0.41              |
| 2:b:5326:ARG:NH2   | 2:b:5442:ILE:CG2   | 2.83                     | 0.41              |
| 2:b:5341:LYS:O     | 2:b:5404:GLY:HA3   | 2.20                     | 0.41              |
| 2:b:5370:LEU:HD12  | 2:b:5370:LEU:N     | 2.35                     | 0.41              |
| 2:b:5445:THR:OG1   | 2:b:5449:GLY:HA3   | 2.20                     | 0.41              |
| 22:b:6011:CLA:H42  | 22:b:6011:CLA:O2A  | 2.19                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5309:ALA:C     | 3:c:5311:GLN:N     | 2.78                     | 0.41              |
| 3:c:5309:ALA:O     | 3:c:5311:GLN:N     | 2.53                     | 0.41              |
| 22:c:6031:CLA:OBD  | 22:c:6033:CLA:C15  | 2.68                     | 0.41              |
| 22:c:6031:CLA:H121 | 22:c:6031:CLA:H161 | 1.62                     | 0.41              |
| 29:c:6056:DGD:HB32 | 29:c:6057:DGD:HA31 | 2.01                     | 0.41              |
| 4:d:5067:TYR:CE1   | 4:d:5076:VAL:HG11  | 2.55                     | 0.41              |
| 4:d:5210:LEU:HD12  | 4:d:5210:LEU:HA    | 1.64                     | 0.41              |
| 5:e:5023:HIS:O     | 5:e:5027:ILE:HD13  | 2.21                     | 0.41              |
| 5:e:5074:GLN:O     | 5:e:5077:GLU:HB2   | 2.20                     | 0.41              |
| 13:o:5192:SER:OG   | 13:o:5193:GLY:N    | 2.53                     | 0.41              |
| 13:o:5197:ALA:O    | 13:o:5199:ALA:N    | 2.53                     | 0.41              |
| 16:v:5156:TRP:HA   | 16:v:5156:TRP:CE3  | 2.55                     | 0.41              |
| 1:A:107:TYR:O      | 1:A:109:GLY:N      | 2.53                     | 0.41              |
| 1:A:142:TRP:CZ2    | 1:A:273:PHE:HD1    | 2.38                     | 0.41              |
| 1:A:183:MET:CB     | 22:A:1003:CLA:HBC3 | 2.35                     | 0.41              |
| 1:A:309:ALA:C      | 1:A:311:GLY:N      | 2.77                     | 0.41              |
| 2:B:36:SER:O       | 2:B:37:MET:C       | 2.63                     | 0.41              |
| 2:B:90:PHE:CD2     | 2:B:90:PHE:O       | 2.74                     | 0.41              |
| 2:B:191:ASN:O      | 2:B:194:ASN:N      | 2.52                     | 0.41              |
| 2:B:246:PHE:C      | 2:B:246:PHE:HD1    | 2.28                     | 0.41              |
| 2:B:280:PHE:O      | 2:B:284:ILE:CG1    | 2.67                     | 0.41              |
| 2:B:326:ARG:HG2    | 4:D:297:ASP:OD2    | 2.20                     | 0.41              |
| 22:B:1016:CLA:H112 | 22:B:1016:CLA:H142 | 1.63                     | 0.41              |
| 25:B:1047:BCR:H23C | 25:t:1046:BCR:C35  | 2.50                     | 0.41              |
| 3:C:187:ASP:C      | 3:C:187:ASP:OD2    | 2.62                     | 0.41              |
| 3:C:343:ARG:HH11   | 3:C:348:GLU:CG     | 2.24                     | 0.41              |
| 3:C:422:PRO:O      | 3:C:426:LEU:HD13   | 2.20                     | 0.41              |
| 3:C:432:VAL:HG13   | 3:C:433:LEU:N      | 2.35                     | 0.41              |
| 4:D:153:PHE:O      | 4:D:157:PHE:HB2    | 2.20                     | 0.41              |
| 4:D:313:THR:H      | 4:D:316:THR:CG2    | 2.34                     | 0.41              |
| 4:D:315:TYR:CZ     | 4:D:319:LEU:HD12   | 2.55                     | 0.41              |
| 22:D:1005:CLA:HMA2 | 24:D:1042:PQ9:H443 | 2.01                     | 0.41              |
| 22:D:1004:CLA:H111 | 22:D:1004:CLA:H71  | 1.71                     | 0.41              |
| 6:F:37:ILE:C       | 6:F:39:ALA:N       | 2.74                     | 0.41              |
| 6:F:43:ILE:O       | 9:J:36:LEU:HG      | 2.20                     | 0.41              |
| 11:L:25:LEU:HB3    | 14:T:13:ILE:HG12   | 2.01                     | 0.41              |
| 13:O:183:LEU:HA    | 13:O:188:ARG:O     | 2.21                     | 0.41              |
| 15:U:41:LEU:HD11   | 15:U:74:ILE:CG2    | 2.50                     | 0.41              |
| 15:U:43:PRO:CG     | 16:V:109:ASP:CB    | 2.99                     | 0.41              |
| 15:U:70:ARG:O      | 15:U:71:GLN:C      | 2.64                     | 0.41              |
| 1:a:5052:PHE:HD2   | 1:a:5071:LEU:HD11  | 1.78                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5161:TYR:N     | 1:a:5162:PRO:CD    | 2.83                     | 0.41              |
| 1:a:5180:PHE:O     | 1:a:5184:ILE:CD1   | 2.68                     | 0.41              |
| 1:a:5184:ILE:CD1   | 4:d:5186:GLN:NE2   | 2.84                     | 0.41              |
| 1:a:5213:ALA:HB3   | 23:d:6039:PHO:CBC  | 2.50                     | 0.41              |
| 26:a:6063:LHG:H332 | 26:a:6063:LHG:H302 | 1.58                     | 0.41              |
| 2:b:5062:VAL:HG11  | 22:b:6013:CLA:HED2 | 1.99                     | 0.41              |
| 2:b:5191:ASN:ND2   | 7:h:5060:VAL:CG1   | 2.72                     | 0.41              |
| 22:b:6016:CLA:H8   | 22:h:6017:CLA:H111 | 2.02                     | 0.41              |
| 3:c:5151:TRP:O     | 3:c:5152:LYS:C     | 2.62                     | 0.41              |
| 22:c:6036:CLA:H3A  | 22:c:6036:CLA:HBA1 | 1.59                     | 0.41              |
| 4:d:5031:GLY:O     | 4:d:5033:SER:N     | 2.54                     | 0.41              |
| 4:d:5054:PHE:HD1   | 5:e:5047:PHE:HE1   | 1.69                     | 0.41              |
| 4:d:5183:LEU:O     | 4:d:5184:PHE:C     | 2.62                     | 0.41              |
| 4:d:5247:VAL:C     | 4:d:5249:ALA:N     | 2.78                     | 0.41              |
| 4:d:5276:VAL:HG23  | 4:d:5277:THR:H     | 1.83                     | 0.41              |
| 22:d:6005:CLA:HBD  | 22:d:6005:CLA:HAA1 | 2.01                     | 0.41              |
| 13:o:5076:PHE:CE2  | 13:o:5132:VAL:HG21 | 2.45                     | 0.41              |
| 13:o:5136:MET:HB2  | 13:o:5140:GLU:HB2  | 2.02                     | 0.41              |
| 13:o:5179:THR:CG2  | 13:o:5180:ALA:N    | 2.63                     | 0.41              |
| 20:z:5043:GLY:O    | 20:z:5047:TRP:HB2  | 2.20                     | 0.41              |
| 20:z:5055:GLY:C    | 20:z:5057:LEU:N    | 2.78                     | 0.41              |
| 1:A:60:ILE:O       | 1:A:61:ASP:C       | 2.63                     | 0.41              |
| 1:A:193:LEU:O      | 4:D:179:PHE:CE2    | 2.73                     | 0.41              |
| 1:A:202:VAL:HA     | 1:A:205:VAL:HG11   | 2.02                     | 0.41              |
| 1:A:223:LEU:CG     | 4:D:265:ARG:HG2    | 2.51                     | 0.41              |
| 1:A:271:LEU:C      | 1:A:273:PHE:N      | 2.76                     | 0.41              |
| 2:B:33:TRP:HH2     | 2:B:62:VAL:CG2     | 2.33                     | 0.41              |
| 2:B:98:LEU:O       | 2:B:102:VAL:HG22   | 2.20                     | 0.41              |
| 2:B:247:PHE:O      | 2:B:247:PHE:CD1    | 2.72                     | 0.41              |
| 22:B:1010:CLA:H93  | 22:B:1010:CLA:H62  | 1.81                     | 0.41              |
| 3:C:168:LEU:HB3    | 22:C:1025:CLA:HMC2 | 2.02                     | 0.41              |
| 3:C:200:THR:OG1    | 3:C:201:ASN:N      | 2.53                     | 0.41              |
| 3:C:304:PRO:HG3    | 3:C:398:HIS:O      | 2.21                     | 0.41              |
| 3:C:318:LEU:HD23   | 3:C:318:LEU:C      | 2.45                     | 0.41              |
| 3:C:348:GLU:CB     | 13:O:42:ALA:HB3    | 2.49                     | 0.41              |
| 3:C:350:ILE:CG2    | 3:C:359:TRP:HB2    | 2.31                     | 0.41              |
| 3:C:367:GLU:O      | 3:C:368:PRO:C      | 2.61                     | 0.41              |
| 3:C:431:PHE:CD2    | 3:C:431:PHE:O      | 2.69                     | 0.41              |
| 3:C:443:TRP:CE3    | 3:C:443:TRP:CA     | 3.02                     | 0.41              |
| 22:C:1025:CLA:H203 | 22:C:1025:CLA:H162 | 1.72                     | 0.41              |
| 4:D:27:PHE:HD1     | 6:F:19:ARG:HG3     | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:78:VAL:CG1     | 4:D:173:PHE:CB     | 2.99                     | 0.41              |
| 4:D:87:HIS:C       | 4:D:167:TRP:NE1    | 2.78                     | 0.41              |
| 4:D:116:LEU:O      | 4:D:120:PHE:CD2    | 2.74                     | 0.41              |
| 4:D:273:PHE:O      | 4:D:276:VAL:HG22   | 2.21                     | 0.41              |
| 4:D:282:SER:HB2    | 22:D:1004:CLA:HED3 | 2.01                     | 0.41              |
| 22:D:1008:CLA:H61  | 22:D:1008:CLA:H41  | 1.64                     | 0.41              |
| 6:F:34:LEU:HD13    | 9:J:28:PHE:HZ      | 1.85                     | 0.41              |
| 28:L:1061:MGE:H6B2 | 28:L:1061:MGE:H3B1 | 1.58                     | 0.41              |
| 13:O:33:TYR:CD2    | 13:O:33:TYR:C      | 2.98                     | 0.41              |
| 13:O:56:TYR:O      | 13:O:161:SER:HA    | 2.20                     | 0.41              |
| 13:O:195:ASP:OD1   | 13:O:195:ASP:C     | 2.62                     | 0.41              |
| 14:T:22:PHE:N      | 14:T:22:PHE:HD1    | 2.17                     | 0.41              |
| 16:V:105:PRO:HG2   | 16:V:115:ALA:CA    | 2.50                     | 0.41              |
| 1:a:5120:LEU:HD11  | 1:a:5155:PHE:CD1   | 2.55                     | 0.41              |
| 1:a:5142:TRP:CZ2   | 1:a:5273:PHE:HD1   | 2.38                     | 0.41              |
| 1:a:5193:LEU:O     | 4:d:5179:PHE:CE2   | 2.73                     | 0.41              |
| 1:a:5202:VAL:HA    | 1:a:5205:VAL:HG11  | 2.02                     | 0.41              |
| 1:a:5223:LEU:CD1   | 4:d:5265:ARG:HG2   | 2.46                     | 0.41              |
| 23:a:6038:PHO:HAA1 | 23:a:6038:PHO:HBD  | 2.02                     | 0.41              |
| 23:a:6038:PHO:OBD  | 23:a:6038:PHO:O2D  | 2.38                     | 0.41              |
| 2:b:5018:ARG:HH11  | 11:l:5004:ASN:ND2  | 2.19                     | 0.41              |
| 2:b:5041:GLU:CD    | 2:b:5062:VAL:H     | 2.28                     | 0.41              |
| 2:b:5113:TRP:CZ2   | 22:b:6024:CLA:HBD  | 2.56                     | 0.41              |
| 2:b:5284:ILE:HD11  | 2:b:5309:LEU:HG    | 2.01                     | 0.41              |
| 2:b:5469:HIS:O     | 2:b:5473:THR:N     | 2.54                     | 0.41              |
| 22:b:6024:CLA:H111 | 22:b:6024:CLA:H143 | 1.77                     | 0.41              |
| 3:c:5064:ALA:O     | 3:c:5068:THR:CB    | 2.68                     | 0.41              |
| 3:c:5222:GLY:HA3   | 3:c:5225:VAL:HG22  | 2.03                     | 0.41              |
| 3:c:5229:ASN:ND2   | 3:c:5232:ASP:OD2   | 2.47                     | 0.41              |
| 3:c:5315:MET:HE2   | 3:c:5319:ILE:CG1   | 2.50                     | 0.41              |
| 4:d:5078:VAL:CG1   | 4:d:5173:PHE:CB    | 2.99                     | 0.41              |
| 4:d:5093:TRP:HA    | 4:d:5099:GLY:H     | 1.84                     | 0.41              |
| 4:d:5111:TRP:CE2   | 4:d:5173:PHE:HE2   | 2.38                     | 0.41              |
| 4:d:5275:PRO:HB2   | 4:d:5276:VAL:H     | 1.66                     | 0.41              |
| 28:d:6062:MGE:O1A  | 28:d:6062:MGE:C4B  | 2.66                     | 0.41              |
| 13:o:5183:LEU:HA   | 13:o:5188:ARG:O    | 2.21                     | 0.41              |
| 17:x:5012:ILE:O    | 17:x:5012:ILE:CG1  | 2.67                     | 0.41              |
| 1:A:14:TRP:C       | 1:A:14:TRP:HD1     | 2.29                     | 0.41              |
| 1:A:121:LEU:C      | 1:A:123:ALA:H      | 2.29                     | 0.41              |
| 1:A:172:MET:HE3    | 1:A:182:PHE:CD2    | 2.40                     | 0.41              |
| 1:A:185:VAL:HG12   | 1:A:186:PHE:N      | 2.34                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:190:HIS:HA     | 1:A:298:ASN:HB3    | 2.03                     | 0.41              |
| 1:A:207:GLY:O      | 1:A:208:GLY:C      | 2.64                     | 0.41              |
| 1:A:272:HIS:HB3    | 4:D:218:VAL:CG1    | 2.50                     | 0.41              |
| 24:A:1043:PQ9:H37  | 24:A:1043:PQ9:H311 | 2.01                     | 0.41              |
| 2:B:113:TRP:CZ2    | 22:B:1024:CLA:HBD  | 2.56                     | 0.41              |
| 2:B:147:GLY:O      | 2:B:148:LEU:C      | 2.64                     | 0.41              |
| 2:B:172:TYR:CD2    | 2:B:173:GLY:N      | 2.88                     | 0.41              |
| 2:B:201:HIS:CD2    | 2:B:202:HIS:CD2    | 3.09                     | 0.41              |
| 2:B:333:GLY:HA2    | 2:B:442:ILE:O      | 2.20                     | 0.41              |
| 2:B:366:PHE:CG     | 2:B:367:PRO:HD2    | 2.56                     | 0.41              |
| 22:B:1023:CLA:HAA2 | 22:B:1023:CLA:CBD  | 2.51                     | 0.41              |
| 22:B:1024:CLA:O2A  | 22:B:1024:CLA:C2A  | 2.62                     | 0.41              |
| 3:C:81:MET:O       | 3:C:86:LEU:HD12    | 2.20                     | 0.41              |
| 3:C:101:PRO:C      | 3:C:102:GLY:O      | 2.63                     | 0.41              |
| 3:C:131:TYR:C      | 3:C:133:ALA:N      | 2.77                     | 0.41              |
| 3:C:305:THR:O      | 3:C:308:GLU:HB3    | 2.19                     | 0.41              |
| 25:C:1052:BCR:C8   | 25:C:1052:BCR:H331 | 2.49                     | 0.41              |
| 4:D:176:ALA:O      | 4:D:179:PHE:N      | 2.52                     | 0.41              |
| 4:D:249:ALA:O      | 4:D:250:ASN:C      | 2.63                     | 0.41              |
| 6:F:15:ILE:HD12    | 31:F:1040:HEM:HMD1 | 2.02                     | 0.41              |
| 9:J:34:ALA:O       | 9:J:35:GLY:O       | 2.39                     | 0.41              |
| 13:O:162:ILE:HD13  | 13:O:269:ILE:HD12  | 2.02                     | 0.41              |
| 16:V:32:GLU:HA     | 16:V:35:THR:CB     | 2.51                     | 0.41              |
| 1:a:5059:ASP:O     | 1:a:5061:ASP:O     | 2.39                     | 0.41              |
| 1:a:5173:PRO:HD2   | 1:a:5182:PHE:HB2   | 2.03                     | 0.41              |
| 1:a:5200:LEU:O     | 1:a:5203:ALA:HB3   | 2.21                     | 0.41              |
| 1:a:5316:THR:CG2   | 4:d:5075:THR:HG23  | 2.51                     | 0.41              |
| 1:a:5318:ALA:O     | 1:a:5321:ILE:HB    | 2.21                     | 0.41              |
| 2:b:5219:VAL:HG12  | 2:b:5220:ARG:N     | 2.34                     | 0.41              |
| 2:b:5246:PHE:C     | 2:b:5246:PHE:HD1   | 2.28                     | 0.41              |
| 3:c:5284:PHE:HB3   | 29:c:6055:DGD:C8B  | 2.50                     | 0.41              |
| 3:c:5404:LEU:O     | 3:c:5405:ASN:C     | 2.63                     | 0.41              |
| 3:c:5451:ALA:O     | 3:c:5454:GLY:N     | 2.53                     | 0.41              |
| 3:c:5459:ILE:O     | 4:d:5223:PHE:HA    | 2.21                     | 0.41              |
| 22:c:6025:CLA:H3A  | 22:c:6025:CLA:HBA2 | 1.58                     | 0.41              |
| 22:c:6035:CLA:H93  | 22:c:6035:CLA:H2   | 2.02                     | 0.41              |
| 22:c:6036:CLA:H42  | 22:c:6036:CLA:O2A  | 2.19                     | 0.41              |
| 4:d:5148:ALA:CB    | 4:d:5149:PRO:HD3   | 2.29                     | 0.41              |
| 4:d:5221:THR:CG2   | 4:d:5248:THR:HB    | 2.46                     | 0.41              |
| 5:e:5032:ILE:HD13  | 5:e:5032:ILE:HA    | 1.92                     | 0.41              |
| 22:h:6017:CLA:H61  | 22:h:6017:CLA:H41  | 1.61                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:o:5209:ALA:O    | 13:o:5210:ARG:C    | 2.62                     | 0.41              |
| 14:t:5018:PHE:CD1  | 25:t:1046:BCR:C33  | 2.94                     | 0.41              |
| 15:u:5043:PRO:CG   | 16:v:5109:ASP:CB   | 2.99                     | 0.41              |
| 15:u:5073:GLN:HA   | 15:u:5073:GLN:NE2  | 2.36                     | 0.41              |
| 15:u:5075:LEU:HD12 | 15:u:5075:LEU:N    | 2.34                     | 0.41              |
| 15:u:5078:ASN:O    | 15:u:5079:LEU:C    | 2.61                     | 0.41              |
| 1:A:93:PHE:C       | 1:A:95:PRO:HD3     | 2.45                     | 0.41              |
| 1:A:184:ILE:CD1    | 4:D:186:GLN:NE2    | 2.84                     | 0.41              |
| 1:A:226:GLU:O      | 1:A:227:THR:HB     | 2.21                     | 0.41              |
| 1:A:323:ARG:CG     | 4:D:329:MET:HA     | 2.50                     | 0.41              |
| 22:A:1003:CLA:CHD  | 22:A:1003:CLA:CBC  | 2.96                     | 0.41              |
| 22:A:1007:CLA:H142 | 22:A:1007:CLA:H111 | 1.67                     | 0.41              |
| 2:B:12:LEU:C       | 2:B:13:ILE:CG2     | 2.94                     | 0.41              |
| 2:B:121:GLU:O      | 2:B:124:ARG:N      | 2.35                     | 0.41              |
| 2:B:149:LEU:CB     | 22:B:1012:CLA:C20  | 2.95                     | 0.41              |
| 2:B:346:PHE:HE1    | 2:B:421:ALA:HB2    | 1.84                     | 0.41              |
| 2:B:359:MET:HE2    | 2:B:359:MET:HB2    | 1.92                     | 0.41              |
| 2:B:469:HIS:O      | 2:B:473:THR:N      | 2.54                     | 0.41              |
| 2:B:472:ARG:CD     | 22:B:1019:CLA:HED3 | 2.50                     | 0.41              |
| 22:B:1010:CLA:C3D  | 22:B:1011:CLA:CMB  | 2.98                     | 0.41              |
| 22:B:1018:CLA:H8   | 22:B:1023:CLA:HBA2 | 2.01                     | 0.41              |
| 3:C:33:PHE:CD2     | 4:D:229:ALA:CB     | 3.04                     | 0.41              |
| 3:C:62:PHE:CE2     | 10:K:29:PRO:HG3    | 2.55                     | 0.41              |
| 3:C:131:TYR:C      | 3:C:133:ALA:H      | 2.29                     | 0.41              |
| 3:C:401:LEU:O      | 3:C:409:GLY:N      | 2.48                     | 0.41              |
| 22:C:1026:CLA:H92  | 22:C:1026:CLA:H61  | 1.63                     | 0.41              |
| 4:D:53:THR:HG22    | 4:D:67:TYR:HD2     | 1.85                     | 0.41              |
| 4:D:67:TYR:CE1     | 4:D:76:VAL:HG11    | 2.55                     | 0.41              |
| 4:D:92:LEU:HG      | 4:D:99:GLY:HA2     | 2.03                     | 0.41              |
| 5:E:77:GLU:O       | 5:E:80:LEU:N       | 2.53                     | 0.41              |
| 22:K:1034:CLA:H43  | 22:K:1034:CLA:CBA  | 2.44                     | 0.41              |
| 16:V:118:HIS:NE2   | 31:V:1041:HEM:NB   | 2.69                     | 0.41              |
| 1:a:5129:ARG:CZ    | 4:d:5256:ILE:CD1   | 2.91                     | 0.41              |
| 1:a:5172:MET:HE3   | 1:a:5182:PHE:CD2   | 2.40                     | 0.41              |
| 1:a:5223:LEU:CG    | 4:d:5265:ARG:HG2   | 2.51                     | 0.41              |
| 1:a:5259:ILE:O     | 1:a:5260:PHE:HB2   | 2.20                     | 0.41              |
| 25:a:6044:BCR:C39  | 25:a:6044:BCR:H373 | 2.29                     | 0.41              |
| 2:b:5230:ARG:O     | 2:b:5231:MET:C     | 2.63                     | 0.41              |
| 2:b:5280:PHE:O     | 2:b:5284:ILE:CG1   | 2.67                     | 0.41              |
| 2:b:5326:ARG:HG2   | 4:d:5297:ASP:OD2   | 2.20                     | 0.41              |
| 2:b:5422:ARG:O     | 2:b:5422:ARG:HG2   | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:b:6015:CLA:HAA1 | 22:b:6015:CLA:CBD  | 2.50                     | 0.41              |
| 22:b:6023:CLA:H112 | 22:b:6024:CLA:C11  | 2.51                     | 0.41              |
| 3:c:5079:LYS:O     | 3:c:5084:GLN:NE2   | 2.54                     | 0.41              |
| 3:c:5081:MET:O     | 3:c:5086:LEU:HD12  | 2.20                     | 0.41              |
| 3:c:5109:PHE:CB    | 3:c:5110:PRO:HD3   | 2.46                     | 0.41              |
| 3:c:5418:ASN:HD22  | 29:c:6057:DGD:HE61 | 1.84                     | 0.41              |
| 3:c:5464:GLU:HA    | 3:c:5465:PRO:HD3   | 1.84                     | 0.41              |
| 22:c:6025:CLA:H62  | 22:c:6025:CLA:H93  | 1.59                     | 0.41              |
| 4:d:5021:TRP:CE3   | 4:d:5022:LEU:HB3   | 2.55                     | 0.41              |
| 4:d:5171:PRO:HA    | 4:d:5181:PHE:CE2   | 2.55                     | 0.41              |
| 4:d:5249:ALA:O     | 4:d:5250:ASN:C     | 2.63                     | 0.41              |
| 4:d:5253:TRP:C     | 4:d:5255:GLN:N     | 2.78                     | 0.41              |
| 7:h:5027:THR:HG22  | 22:h:6017:CLA:HMD2 | 2.01                     | 0.41              |
| 11:l:5029:LEU:C    | 11:l:5029:LEU:CD1  | 2.90                     | 0.41              |
| 12:m:5020:VAL:O    | 12:m:5024:ILE:HG13 | 2.20                     | 0.41              |
| 13:o:5056:TYR:O    | 13:o:5161:SER:HA   | 2.21                     | 0.41              |
| 14:t:5002:GLU:N    | 14:t:5002:GLU:OE1  | 2.54                     | 0.41              |
| 16:v:5047:LEU:CG   | 16:v:5048:THR:H    | 2.33                     | 0.41              |
| 16:v:5071:ILE:HG13 | 16:v:5072:THR:N    | 2.35                     | 0.41              |
| 16:v:5108:TYR:O    | 16:v:5108:TYR:CD2  | 2.72                     | 0.41              |
| 17:x:5023:LEU:C    | 17:x:5023:LEU:HD23 | 2.46                     | 0.41              |
| 20:z:5035:ARG:HG3  | 20:z:5036:SER:H    | 1.86                     | 0.41              |
| 1:A:135:TYR:HE1    | 3:C:449:ARG:O      | 2.03                     | 0.41              |
| 1:A:258:LEU:C      | 1:A:259:ILE:CG1    | 2.92                     | 0.41              |
| 25:A:1044:BCR:C37  | 25:A:1044:BCR:C30  | 2.61                     | 0.41              |
| 2:B:12:LEU:CD2     | 2:B:19:LEU:HA      | 2.51                     | 0.41              |
| 2:B:125:ASP:OD1    | 2:B:126:PRO:HD2    | 2.21                     | 0.41              |
| 2:B:242:ILE:HG22   | 2:B:466:HIS:HB2    | 2.03                     | 0.41              |
| 2:B:421:ALA:O      | 2:B:424:ALA:N      | 2.50                     | 0.41              |
| 2:B:429:ILE:HG22   | 2:B:430:PHE:N      | 2.34                     | 0.41              |
| 22:B:1012:CLA:HBB1 | 22:B:1015:CLA:CAB  | 2.45                     | 0.41              |
| 22:B:1013:CLA:C2B  | 22:B:1014:CLA:H11  | 2.51                     | 0.41              |
| 22:B:1016:CLA:CHD  | 22:B:1016:CLA:CBC  | 2.97                     | 0.41              |
| 22:B:1019:CLA:C19  | 22:B:1021:CLA:H71  | 2.50                     | 0.41              |
| 22:B:1023:CLA:H112 | 22:B:1024:CLA:C11  | 2.51                     | 0.41              |
| 3:C:110:PRO:O      | 3:C:113:VAL:HB     | 2.21                     | 0.41              |
| 3:C:309:ALA:C      | 3:C:311:GLN:N      | 2.78                     | 0.41              |
| 3:C:315:MET:HA     | 3:C:315:MET:CE     | 2.43                     | 0.41              |
| 22:C:1028:CLA:H71  | 22:C:1028:CLA:H111 | 1.83                     | 0.41              |
| 4:D:42:TYR:O       | 4:D:43:LEU:C       | 2.64                     | 0.41              |
| 4:D:161:PRO:HG3    | 4:D:170:ALA:HA     | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:186:GLN:CB     | 22:D:1004:CLA:HBC1 | 2.51                     | 0.41              |
| 4:D:236:ASN:HA     | 4:D:237:PRO:HD2    | 1.96                     | 0.41              |
| 4:D:267:LEU:HD23   | 4:D:268:HIS:N      | 2.35                     | 0.41              |
| 5:E:23:HIS:O       | 5:E:27:ILE:HD13    | 2.21                     | 0.41              |
| 5:E:34:GLY:CA      | 6:F:32:PHE:CD1     | 3.03                     | 0.41              |
| 11:L:19:LEU:N      | 11:L:19:LEU:HD23   | 2.34                     | 0.41              |
| 20:Z:43:GLY:O      | 20:Z:47:TRP:HB2    | 2.20                     | 0.41              |
| 1:a:5037:MET:SD    | 1:a:5126:TYR:CB    | 3.08                     | 0.41              |
| 1:a:5055:ALA:O     | 1:a:5073:TYR:CD2   | 2.74                     | 0.41              |
| 1:a:5121:LEU:C     | 1:a:5123:ALA:H     | 2.29                     | 0.41              |
| 1:a:5127:MET:C     | 1:a:5130:GLN:HB3   | 2.42                     | 0.41              |
| 1:a:5141:PRO:HG2   | 3:c:5446:GLY:O     | 2.21                     | 0.41              |
| 1:a:5262:TYR:C     | 1:a:5264:SER:H     | 2.27                     | 0.41              |
| 22:a:6006:CLA:HAA1 | 22:a:6006:CLA:CBD  | 2.50                     | 0.41              |
| 2:b:5055:MET:O     | 2:b:5057:ARG:N     | 2.54                     | 0.41              |
| 2:b:5429:ILE:N     | 2:b:5429:ILE:CD1   | 2.76                     | 0.41              |
| 22:b:6021:CLA:HED3 | 22:b:6021:CLA:C2   | 2.41                     | 0.41              |
| 22:b:6021:CLA:HED1 | 22:b:6021:CLA:H52  | 2.02                     | 0.41              |
| 22:c:6033:CLA:C9   | 22:c:6036:CLA:CAA  | 2.97                     | 0.41              |
| 4:d:5042:TYR:O     | 4:d:5043:LEU:C     | 2.64                     | 0.41              |
| 4:d:5103:ARG:HG3   | 5:e:5073:LYS:CD    | 2.50                     | 0.41              |
| 4:d:5116:LEU:O     | 4:d:5120:PHE:CD2   | 2.74                     | 0.41              |
| 4:d:5140:PRO:C     | 4:d:5142:ASN:N     | 2.79                     | 0.41              |
| 9:j:5034:ALA:O     | 9:j:5035:GLY:C     | 2.64                     | 0.41              |
| 16:v:5047:LEU:HG   | 16:v:5048:THR:H    | 1.86                     | 0.41              |
| 16:v:5061:TYR:C    | 16:v:5063:CYS:H    | 2.28                     | 0.41              |
| 16:v:5118:HIS:NE2  | 31:v:6041:HEM:NB   | 2.69                     | 0.41              |
| 20:z:5058:ASN:C    | 20:z:5060:PHE:N    | 2.77                     | 0.41              |
| 1:A:46:ILE:HD13    | 1:A:46:ILE:HA      | 1.88                     | 0.41              |
| 1:A:120:LEU:HD11   | 1:A:155:PHE:CD1    | 2.55                     | 0.41              |
| 1:A:124:SER:OG     | 1:A:155:PHE:CE2    | 2.74                     | 0.41              |
| 1:A:180:PHE:HD1    | 4:D:192:THR:HB     | 1.73                     | 0.41              |
| 1:A:195:HIS:ND1    | 1:A:197:PHE:HB2    | 2.36                     | 0.41              |
| 1:A:279:ARG:HG2    | 4:D:212:ALA:CB     | 2.50                     | 0.41              |
| 1:A:316:THR:CG2    | 4:D:75:THR:CG2     | 2.99                     | 0.41              |
| 1:A:331:MET:CG     | 4:D:320:LEU:HD22   | 2.51                     | 0.41              |
| 22:A:1006:CLA:HAA2 | 29:C:1057:DGD:HBN2 | 2.02                     | 0.41              |
| 2:B:41:GLU:HB3     | 2:B:60:MET:SD      | 2.60                     | 0.41              |
| 2:B:49:ASP:C       | 2:B:51:VAL:H       | 2.26                     | 0.41              |
| 2:B:62:VAL:C       | 2:B:64:PRO:HD2     | 2.46                     | 0.41              |
| 2:B:67:ALA:CB      | 2:B:267:LEU:HD21   | 2.50                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:69:LEU:HD23    | 22:B:1013:CLA:H3A  | 2.03                     | 0.41              |
| 2:B:110:ALA:O      | 2:B:113:TRP:HB3    | 2.21                     | 0.41              |
| 2:B:121:GLU:HB3    | 7:H:4:ARG:HA       | 2.01                     | 0.41              |
| 2:B:137:LYS:NZ     | 2:B:137:LYS:HB3    | 2.36                     | 0.41              |
| 2:B:185:TRP:C      | 2:B:186:GLY:O      | 2.64                     | 0.41              |
| 2:B:192:PRO:HG3    | 7:H:49:TYR:CD1     | 2.55                     | 0.41              |
| 2:B:219:VAL:HG12   | 2:B:220:ARG:N      | 2.34                     | 0.41              |
| 2:B:271:THR:HG23   | 2:B:274:GLN:H      | 1.85                     | 0.41              |
| 2:B:341:LYS:O      | 2:B:404:GLY:HA3    | 2.20                     | 0.41              |
| 22:B:1011:CLA:H92  | 22:B:1011:CLA:CBB  | 2.43                     | 0.41              |
| 22:B:1016:CLA:H8   | 22:H:1017:CLA:H111 | 2.02                     | 0.41              |
| 3:C:49:LEU:HD23    | 3:C:133:ALA:HB2    | 2.03                     | 0.41              |
| 3:C:284:PHE:HB3    | 29:C:1055:DGD:C8B  | 2.50                     | 0.41              |
| 3:C:376:ASP:OD1    | 3:C:379:LYS:HG3    | 2.20                     | 0.41              |
| 3:C:386:PRO:C      | 3:C:388:GLN:H      | 2.28                     | 0.41              |
| 22:C:1025:CLA:H3A  | 22:C:1025:CLA:HBA2 | 1.58                     | 0.41              |
| 29:C:1056:DGD:HG12 | 29:C:1056:DGD:HB21 | 2.02                     | 0.41              |
| 4:D:89:LEU:O       | 4:D:90:LEU:C       | 2.63                     | 0.41              |
| 4:D:103:ARG:HG3    | 5:E:73:LYS:CD      | 2.50                     | 0.41              |
| 4:D:129:GLN:NE2    | 4:D:142:ASN:OD1    | 2.54                     | 0.41              |
| 22:D:1005:CLA:CMA  | 24:D:1042:PQ9:H443 | 2.50                     | 0.41              |
| 23:D:1039:PHO:H92  | 23:D:1039:PHO:H111 | 1.74                     | 0.41              |
| 25:D:1050:BCR:C16  | 25:D:1050:BCR:H351 | 2.48                     | 0.41              |
| 6:F:13:TYR:HA      | 6:F:14:PRO:HD3     | 1.96                     | 0.41              |
| 13:O:37:VAL:O      | 13:O:37:VAL:CG1    | 2.68                     | 0.41              |
| 13:O:118:SER:HB3   | 13:O:157:PRO:HA    | 2.03                     | 0.41              |
| 13:O:131:PRO:HA    | 13:O:145:LEU:HD12  | 2.03                     | 0.41              |
| 13:O:184:ASP:CG    | 13:O:188:ARG:HH12  | 2.29                     | 0.41              |
| 13:O:188:ARG:HD3   | 13:O:212:ASN:OD1   | 2.21                     | 0.41              |
| 13:O:211:ALA:O     | 13:O:214:LYS:HD3   | 2.21                     | 0.41              |
| 13:O:265:PHE:HD1   | 13:O:266:TYR:O     | 2.04                     | 0.41              |
| 16:V:35:THR:HG23   | 16:V:46:THR:H      | 1.85                     | 0.41              |
| 16:V:70:GLY:HA3    | 16:V:156:TRP:CE3   | 2.56                     | 0.41              |
| 20:Z:35:ARG:HG3    | 20:Z:36:SER:H      | 1.86                     | 0.41              |
| 1:a:5076:ASN:HB2   | 1:a:5079:THR:CG2   | 2.51                     | 0.41              |
| 1:a:5085:SER:OG    | 1:a:5168:PHE:HB2   | 2.21                     | 0.41              |
| 1:a:5104:GLU:O     | 1:a:5105:TRP:C     | 2.63                     | 0.41              |
| 1:a:5107:TYR:O     | 1:a:5109:GLY:N     | 2.53                     | 0.41              |
| 1:a:5124:SER:OG    | 1:a:5155:PHE:CE2   | 2.74                     | 0.41              |
| 1:a:5147:TYR:CA    | 23:a:6038:PHO:HMD2 | 2.50                     | 0.41              |
| 1:a:5150:PRO:C     | 22:a:6003:CLA:H52  | 2.46                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5187:GLN:HG2   | 1:a:5328:MET:HE1   | 2.02                     | 0.41              |
| 1:a:5190:HIS:HA    | 1:a:5298:ASN:HB3   | 2.03                     | 0.41              |
| 1:a:5193:LEU:O     | 1:a:5193:LEU:CD2   | 2.68                     | 0.41              |
| 1:a:5226:GLU:O     | 1:a:5227:THR:HB    | 2.21                     | 0.41              |
| 1:a:5318:ALA:HA    | 1:a:5321:ILE:CD1   | 2.50                     | 0.41              |
| 1:a:5338:ASN:C     | 1:a:5339:PHE:CG    | 2.99                     | 0.41              |
| 22:a:6003:CLA:CHD  | 22:a:6003:CLA:CBC  | 2.96                     | 0.41              |
| 23:a:6038:PHO:CHD  | 4:d:5209:LEU:HG    | 2.51                     | 0.41              |
| 2:b:5012:LEU:C     | 2:b:5014:ASN:N     | 2.79                     | 0.41              |
| 2:b:5024:LEU:CG    | 2:b:5111:ALA:HA    | 2.50                     | 0.41              |
| 2:b:5042:LEU:HD12  | 2:b:5042:LEU:HA    | 1.95                     | 0.41              |
| 2:b:5066:MET:O     | 2:b:5071:VAL:N     | 2.54                     | 0.41              |
| 2:b:5095:GLY:O     | 2:b:5096:VAL:C     | 2.64                     | 0.41              |
| 2:b:5137:LYS:NZ    | 2:b:5137:LYS:HB3   | 2.36                     | 0.41              |
| 2:b:5292:LEU:C     | 2:b:5294:SER:N     | 2.79                     | 0.41              |
| 2:b:5306:PRO:O     | 2:b:5307:GLU:C     | 2.64                     | 0.41              |
| 2:b:5308:LYS:O     | 2:b:5312:TYR:CD2   | 2.74                     | 0.41              |
| 2:b:5333:GLY:HA2   | 2:b:5442:ILE:O     | 2.21                     | 0.41              |
| 2:b:5366:PHE:CG    | 2:b:5367:PRO:HD2   | 2.55                     | 0.41              |
| 2:b:5392:PHE:HE2   | 2:b:5417:VAL:HG12  | 1.85                     | 0.41              |
| 2:b:5468:TRP:CZ2   | 22:b:6019:CLA:HED2 | 2.56                     | 0.41              |
| 2:b:5478:VAL:O     | 2:b:5479:PHE:C     | 2.64                     | 0.41              |
| 22:b:6018:CLA:H141 | 22:b:6018:CLA:OBD  | 2.21                     | 0.41              |
| 22:b:6022:CLA:H202 | 22:b:6022:CLA:C3D  | 2.49                     | 0.41              |
| 28:b:6060:MGE:H7A1 | 28:b:6060:MGE:H121 | 2.03                     | 0.41              |
| 3:c:5118:HIS:HA    | 3:c:5121:SER:HB3   | 2.03                     | 0.41              |
| 3:c:5157:MET:HE2   | 3:c:5271:TYR:CE2   | 2.55                     | 0.41              |
| 3:c:5200:THR:OG1   | 3:c:5201:ASN:N     | 2.53                     | 0.41              |
| 3:c:5340:TYR:C     | 3:c:5341:LEU:HG    | 2.46                     | 0.41              |
| 3:c:5343:ARG:NH1   | 3:c:5348:GLU:CB    | 2.82                     | 0.41              |
| 3:c:5343:ARG:NH2   | 13:o:5103:SER:O    | 2.47                     | 0.41              |
| 3:c:5425:TRP:CD1   | 22:c:6028:CLA:HMA2 | 2.55                     | 0.41              |
| 4:d:5053:THR:HG23  | 4:d:5067:TYR:HE2   | 1.83                     | 0.41              |
| 4:d:5090:LEU:HD12  | 4:d:5096:GLU:CG    | 2.49                     | 0.41              |
| 4:d:5097:ALA:HB1   | 4:d:5104:TRP:HB2   | 2.01                     | 0.41              |
| 4:d:5098:GLN:O     | 4:d:5099:GLY:C     | 2.63                     | 0.41              |
| 4:d:5284:ILE:O     | 4:d:5287:VAL:N     | 2.54                     | 0.41              |
| 4:d:5307:GLU:H     | 4:d:5307:GLU:HG3   | 1.57                     | 0.41              |
| 6:f:5028:VAL:CB    | 6:f:5029:PRO:HD3   | 2.41                     | 0.41              |
| 7:h:5002:ALA:O     | 7:h:5003:ARG:HB2   | 2.21                     | 0.41              |
| 7:h:5006:TRP:HD1   | 7:h:5010:ILE:HD11  | 1.72                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:h:5027:THR:C     | 22:h:6017:CLA:OBD  | 2.63                     | 0.41              |
| 8:i:5003:THR:O     | 8:i:5006:ILE:HG13  | 2.20                     | 0.41              |
| 10:k:5029:PRO:O    | 10:k:5032:PHE:HB2  | 2.20                     | 0.41              |
| 11:l:5015:THR:HA   | 11:l:5018:TYR:HD2  | 1.86                     | 0.41              |
| 13:o:5172:PHE:HD1  | 13:o:5221:GLY:HA3  | 1.77                     | 0.41              |
| 13:o:5184:ASP:CG   | 13:o:5188:ARG:HB2  | 2.46                     | 0.41              |
| 13:o:5211:ALA:O    | 13:o:5214:LYS:HD3  | 2.21                     | 0.41              |
| 13:o:5223:ILE:HD13 | 13:o:5225:LEU:CD1  | 2.50                     | 0.41              |
| 15:u:5041:LEU:HD11 | 15:u:5074:ILE:CG2  | 2.50                     | 0.41              |
| 15:u:5070:ARG:O    | 15:u:5071:GLN:C    | 2.64                     | 0.41              |
| 16:v:5047:LEU:HD23 | 16:v:5048:THR:O    | 2.21                     | 0.41              |
| 16:v:5070:GLY:HA3  | 16:v:5156:TRP:CE3  | 2.56                     | 0.41              |
| 16:v:5105:PRO:HG2  | 16:v:5115:ALA:CA   | 2.50                     | 0.41              |
| 16:v:5120:SER:O    | 16:v:5123:SER:C    | 2.64                     | 0.41              |
| 16:v:5148:GLU:O    | 16:v:5151:ILE:CD1  | 2.68                     | 0.41              |
| 16:v:5156:TRP:HA   | 16:v:5156:TRP:HE3  | 1.85                     | 0.41              |
| 18:y:5035:ILE:CD1  | 18:y:5036:ILE:HD12 | 2.50                     | 0.41              |
| 1:A:47:CYS:HA      | 25:A:1044:BCR:H372 | 2.02                     | 0.41              |
| 1:A:76:ASN:HB2     | 1:A:79:THR:CG2     | 2.51                     | 0.41              |
| 1:A:141:PRO:HG2    | 3:C:446:GLY:O      | 2.21                     | 0.41              |
| 1:A:210:LEU:HD12   | 23:D:1039:PHO:NC   | 2.36                     | 0.41              |
| 1:A:260:PHE:O      | 4:D:27:PHE:HE2     | 2.04                     | 0.41              |
| 1:A:338:ASN:C      | 1:A:339:PHE:CG     | 2.96                     | 0.41              |
| 22:A:1007:CLA:H193 | 22:A:1007:CLA:H162 | 1.73                     | 0.41              |
| 2:B:41:GLU:CD      | 2:B:62:VAL:H       | 2.28                     | 0.41              |
| 2:B:69:LEU:CB      | 22:B:1014:CLA:HMA1 | 2.51                     | 0.41              |
| 2:B:241:SER:C      | 2:B:243:ALA:N      | 2.77                     | 0.41              |
| 2:B:275:TRP:CH2    | 2:B:358:ARG:HD3    | 2.56                     | 0.41              |
| 2:B:341:LYS:HD2    | 2:B:429:ILE:CG2    | 2.51                     | 0.41              |
| 2:B:422:ARG:O      | 2:B:422:ARG:HG2    | 2.21                     | 0.41              |
| 22:B:1021:CLA:HED1 | 22:B:1021:CLA:H52  | 2.02                     | 0.41              |
| 4:D:100:ASP:O      | 4:D:103:ARG:N      | 2.54                     | 0.41              |
| 4:D:253:TRP:C      | 4:D:255:GLN:N      | 2.78                     | 0.41              |
| 4:D:281:MET:CA     | 4:D:281:MET:CE     | 2.97                     | 0.41              |
| 28:D:1062:MGE:H241 | 14:T:13:ILE:HG21   | 2.03                     | 0.41              |
| 8:I:4:LEU:HA       | 8:I:4:LEU:HD12     | 1.79                     | 0.41              |
| 8:I:9:TYR:O        | 8:I:13:THR:N       | 2.36                     | 0.41              |
| 11:L:36:PHE:CD1    | 12:M:7:GLY:HA3     | 2.55                     | 0.41              |
| 13:O:136:MET:HB2   | 13:O:140:GLU:HB2   | 2.02                     | 0.41              |
| 13:O:185:PRO:O     | 13:O:186:LYS:CB    | 2.68                     | 0.41              |
| 13:O:197:ALA:O     | 13:O:199:ALA:N     | 2.53                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:T:2:GLU:N       | 14:T:2:GLU:OE1     | 2.54                     | 0.41              |
| 25:T:6046:BCR:H23C | 25:T:6046:BCR:C40  | 2.36                     | 0.41              |
| 16:V:101:TYR:O     | 16:V:102:MET:C     | 2.63                     | 0.41              |
| 1:a:5049:VAL:O     | 1:a:5053:ILE:HG13  | 2.21                     | 0.41              |
| 1:a:5060:ILE:HD12  | 1:a:5084:PRO:HD2   | 2.03                     | 0.41              |
| 1:a:5071:LEU:HD21  | 1:a:5077:ILE:HD13  | 2.03                     | 0.41              |
| 1:a:5121:LEU:O     | 1:a:5122:GLY:C     | 2.64                     | 0.41              |
| 1:a:5142:TRP:NE1   | 4:d:5219:GLU:HB3   | 2.36                     | 0.41              |
| 1:a:5159:LEU:HD23  | 29:c:6055:DGD:HA82 | 2.03                     | 0.41              |
| 1:a:5207:GLY:O     | 1:a:5208:GLY:C     | 2.64                     | 0.41              |
| 1:a:5215:HIS:HD2   | 1:a:5275:LEU:CD1   | 2.33                     | 0.41              |
| 1:a:5331:MET:CG    | 4:d:5320:LEU:HD22  | 2.51                     | 0.41              |
| 25:a:6044:BCR:C40  | 25:a:6044:BCR:H372 | 2.29                     | 0.41              |
| 2:b:5012:LEU:C     | 2:b:5013:ILE:CG2   | 2.94                     | 0.41              |
| 2:b:5341:LYS:HD2   | 2:b:5429:ILE:CG2   | 2.51                     | 0.41              |
| 2:b:5407:ASN:C     | 2:b:5409:GLN:H     | 2.28                     | 0.41              |
| 22:b:6013:CLA:C2B  | 22:b:6014:CLA:H11  | 2.51                     | 0.41              |
| 22:b:6020:CLA:HBA1 | 22:b:6020:CLA:H3A  | 1.59                     | 0.41              |
| 3:c:5033:PHE:CD2   | 4:d:5229:ALA:CB    | 3.04                     | 0.41              |
| 3:c:5058:GLY:O     | 3:c:5061:VAL:HG12  | 2.21                     | 0.41              |
| 3:c:5348:GLU:CB    | 13:o:5042:ALA:HB3  | 2.49                     | 0.41              |
| 3:c:5386:PRO:C     | 3:c:5388:GLN:H     | 2.28                     | 0.41              |
| 4:d:5021:TRP:CZ3   | 17:x:5037:LEU:CD2  | 3.04                     | 0.41              |
| 4:d:5087:HIS:O     | 4:d:5088:SER:C     | 2.63                     | 0.41              |
| 22:d:6005:CLA:C15  | 22:d:6005:CLA:C20  | 2.97                     | 0.41              |
| 7:h:5040:VAL:HG12  | 7:h:5044:ILE:HG12  | 2.03                     | 0.41              |
| 22:k:6034:CLA:H93  | 22:k:6034:CLA:H62  | 1.77                     | 0.41              |
| 13:o:5033:TYR:CD2  | 13:o:5033:TYR:C    | 2.98                     | 0.41              |
| 13:o:5079:LYS:HE2  | 13:o:5089:ALA:HB3  | 2.01                     | 0.41              |
| 13:o:5079:LYS:HA   | 13:o:5091:PHE:HA   | 2.03                     | 0.41              |
| 1:A:49:VAL:O       | 1:A:53:ILE:HG13    | 2.21                     | 0.40              |
| 1:A:59:ASP:O       | 1:A:61:ASP:O       | 2.39                     | 0.40              |
| 1:A:96:ILE:O       | 1:A:96:ILE:HG22    | 2.20                     | 0.40              |
| 1:A:104:GLU:O      | 1:A:105:TRP:C      | 2.63                     | 0.40              |
| 1:A:155:PHE:CE1    | 29:C:1055:DGD:HBN1 | 2.56                     | 0.40              |
| 1:A:233:ALA:C      | 4:D:265:ARG:HH12   | 2.29                     | 0.40              |
| 1:A:256:GLY:O      | 1:A:261:GLN:CA     | 2.69                     | 0.40              |
| 1:A:309:ALA:HB3    | 16:V:28:GLU:CG     | 2.50                     | 0.40              |
| 23:A:1038:PHO:HAA1 | 23:A:1038:PHO:HBD  | 2.02                     | 0.40              |
| 24:A:1043:PQ9:H37  | 24:A:1043:PQ9:C31  | 2.51                     | 0.40              |
| 24:A:1043:PQ9:H401 | 24:A:1043:PQ9:H361 | 1.70                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:93:PHE:O       | 2:B:94:GLU:C       | 2.64                     | 0.40              |
| 2:B:135:LEU:H      | 2:B:136:PRO:CD     | 2.34                     | 0.40              |
| 2:B:460:LEU:CA     | 29:B:1058:DGD:HAG1 | 2.38                     | 0.40              |
| 22:B:1016:CLA:HAA1 | 22:B:1016:CLA:CBD  | 2.49                     | 0.40              |
| 22:B:1020:CLA:H91  | 22:B:1020:CLA:H112 | 1.56                     | 0.40              |
| 3:C:321:ASP:OD1    | 3:C:340:TYR:CE1    | 2.74                     | 0.40              |
| 3:C:464:GLU:HA     | 3:C:465:PRO:HD3    | 1.84                     | 0.40              |
| 4:D:21:TRP:CZ3     | 17:X:37:LEU:CD2    | 3.04                     | 0.40              |
| 4:D:68:LEU:CA      | 6:F:40:MET:SD      | 3.06                     | 0.40              |
| 4:D:98:GLN:O       | 4:D:99:GLY:C       | 2.63                     | 0.40              |
| 4:D:284:ILE:O      | 4:D:287:VAL:N      | 2.54                     | 0.40              |
| 22:D:1005:CLA:C15  | 22:D:1005:CLA:C20  | 2.97                     | 0.40              |
| 7:H:47:GLU:OE2     | 7:H:52:THR:HG21    | 2.21                     | 0.40              |
| 9:J:21:VAL:CG1     | 9:J:22:ILE:N       | 2.84                     | 0.40              |
| 9:J:24:ILE:HG23    | 9:J:25:VAL:N       | 2.36                     | 0.40              |
| 16:V:30:THR:HB     | 16:V:31:PRO:CD     | 2.52                     | 0.40              |
| 20:Z:5:PHE:HD1     | 20:Z:57:LEU:HD13   | 1.87                     | 0.40              |
| 1:a:5105:TRP:CH2   | 1:a:5111:PRO:HA    | 2.55                     | 0.40              |
| 1:a:5304:HIS:HE1   | 16:v:5163:TYR:O    | 2.03                     | 0.40              |
| 22:a:6006:CLA:HAA2 | 29:c:6057:DGD:HBN2 | 2.02                     | 0.40              |
| 24:a:6043:PQ9:C45  | 28:d:6059:MGE:C8A  | 2.80                     | 0.40              |
| 24:a:6043:PQ9:H212 | 23:d:6039:PHO:CED  | 2.45                     | 0.40              |
| 2:b:5113:TRP:CD1   | 2:b:5113:TRP:C     | 2.98                     | 0.40              |
| 2:b:5219:VAL:CG1   | 2:b:5220:ARG:N     | 2.84                     | 0.40              |
| 2:b:5248:ALA:CB    | 22:b:6011:CLA:H51  | 2.51                     | 0.40              |
| 2:b:5271:THR:HG23  | 2:b:5274:GLN:H     | 1.85                     | 0.40              |
| 2:b:5421:ALA:O     | 2:b:5424:ALA:N     | 2.50                     | 0.40              |
| 3:c:5131:TYR:C     | 3:c:5133:ALA:H     | 2.29                     | 0.40              |
| 3:c:5173:LEU:O     | 3:c:5174:LEU:C     | 2.63                     | 0.40              |
| 3:c:5304:PRO:HG3   | 3:c:5398:HIS:O     | 2.21                     | 0.40              |
| 22:c:6031:CLA:CMA  | 22:c:6031:CLA:C2   | 2.99                     | 0.40              |
| 29:c:6056:DGD:HAT1 | 29:c:6056:DGD:C6A  | 2.47                     | 0.40              |
| 4:d:5129:GLN:NE2   | 4:d:5142:ASN:OD1   | 2.54                     | 0.40              |
| 4:d:5260:ALA:HA    | 24:d:6042:PQ9:H91  | 2.02                     | 0.40              |
| 4:d:5292:ASN:O     | 4:d:5294:ARG:HG2   | 2.20                     | 0.40              |
| 28:d:6062:MGE:O1G  | 28:d:6062:MGE:C1B  | 2.69                     | 0.40              |
| 7:h:5003:ARG:HE    | 7:h:5003:ARG:HB3   | 1.54                     | 0.40              |
| 9:j:5021:VAL:CG1   | 9:j:5022:ILE:N     | 2.84                     | 0.40              |
| 22:k:6034:CLA:C4   | 22:k:6034:CLA:HBA1 | 2.49                     | 0.40              |
| 1:A:78:ILE:HD13    | 11:L:33:SER:CB     | 2.50                     | 0.40              |
| 1:A:85:SER:OG      | 1:A:168:PHE:HB2    | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:186:PHE:O      | 1:A:189:GLU:N      | 2.54                     | 0.40              |
| 1:A:218:LEU:O      | 1:A:221:SER:N      | 2.52                     | 0.40              |
| 1:A:339:PHE:HB3    | 3:C:313:GLN:CD     | 2.45                     | 0.40              |
| 2:B:5:TRP:CE2      | 28:L:1061:MGE:C2A  | 3.04                     | 0.40              |
| 2:B:19:LEU:O       | 2:B:22:ALA:N       | 2.53                     | 0.40              |
| 2:B:24:LEU:HD22    | 2:B:114:HIS:CD2    | 2.55                     | 0.40              |
| 2:B:52:LEU:CD1     | 2:B:339:ALA:HA     | 2.49                     | 0.40              |
| 2:B:66:MET:O       | 2:B:71:VAL:N       | 2.54                     | 0.40              |
| 2:B:102:VAL:O      | 2:B:106:LEU:HG     | 2.22                     | 0.40              |
| 2:B:106:LEU:O      | 2:B:109:LEU:N      | 2.48                     | 0.40              |
| 2:B:279:TYR:C      | 2:B:279:TYR:CD1    | 2.99                     | 0.40              |
| 2:B:306:PRO:O      | 2:B:307:GLU:C      | 2.64                     | 0.40              |
| 2:B:321:LYS:NZ     | 2:B:321:LYS:HA     | 2.37                     | 0.40              |
| 2:B:392:PHE:CE2    | 2:B:418:LYS:HA     | 2.55                     | 0.40              |
| 3:C:65:GLY:HA3     | 3:C:119:LEU:CA     | 2.51                     | 0.40              |
| 3:C:418:ASN:HD22   | 29:C:1057:DGD:HE61 | 1.84                     | 0.40              |
| 22:C:1027:CLA:H3A  | 22:C:1027:CLA:CGA  | 2.50                     | 0.40              |
| 25:C:1054:BCR:HC8  | 25:C:1054:BCR:C31  | 2.51                     | 0.40              |
| 4:D:21:TRP:CZ3     | 17:X:37:LEU:HD21   | 2.55                     | 0.40              |
| 4:D:100:ASP:C      | 4:D:102:THR:N      | 2.80                     | 0.40              |
| 4:D:199:MET:HG2    | 24:D:1042:PQ9:H352 | 2.02                     | 0.40              |
| 28:D:1062:MGE:O1G  | 28:D:1062:MGE:C1B  | 2.69                     | 0.40              |
| 13:O:79:LYS:HA     | 13:O:91:PHE:HA     | 2.03                     | 0.40              |
| 13:O:183:LEU:CD1   | 13:O:183:LEU:N     | 2.84                     | 0.40              |
| 14:T:14:ILE:CG2    | 14:T:15:ALA:N      | 2.84                     | 0.40              |
| 25:T:6046:BCR:C23  | 25:T:6046:BCR:C39  | 2.83                     | 0.40              |
| 16:V:120:SER:O     | 16:V:123:SER:C     | 2.64                     | 0.40              |
| 16:V:147:VAL:C     | 16:V:149:PRO:HD2   | 2.46                     | 0.40              |
| 1:a:5046:ILE:HD13  | 1:a:5046:ILE:HA    | 1.88                     | 0.40              |
| 1:a:5186:PHE:O     | 1:a:5189:GLU:N     | 2.54                     | 0.40              |
| 2:b:5023:HIS:CD2   | 22:b:6020:CLA:HBA2 | 2.57                     | 0.40              |
| 2:b:5046:ASP:OD1   | 2:b:5048:SER:OG    | 2.39                     | 0.40              |
| 2:b:5125:ASP:OD1   | 2:b:5126:PRO:HD2   | 2.21                     | 0.40              |
| 2:b:5185:TRP:C     | 2:b:5186:GLY:O     | 2.64                     | 0.40              |
| 2:b:5237:VAL:HG12  | 22:b:6020:CLA:HMD1 | 2.03                     | 0.40              |
| 2:b:5272:ARG:NH2   | 2:b:5276:ASP:OD2   | 2.50                     | 0.40              |
| 22:b:6016:CLA:CAB  | 4:d:5123:ILE:HG23  | 2.51                     | 0.40              |
| 29:b:6058:DGD:HG11 | 7:h:5050:ASN:HD22  | 1.84                     | 0.40              |
| 3:c:5289:PHE:C     | 3:c:5289:PHE:CD2   | 2.99                     | 0.40              |
| 3:c:5321:ASP:OD1   | 3:c:5340:TYR:CE1   | 2.74                     | 0.40              |
| 3:c:5322:GLN:HB2   | 3:c:5328:VAL:HG21  | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5377:LEU:C     | 3:c:5377:LEU:CD1   | 2.92                     | 0.40              |
| 3:c:5432:VAL:HG13  | 3:c:5433:LEU:N     | 2.35                     | 0.40              |
| 22:c:6031:CLA:CMD  | 22:c:6033:CLA:C16  | 2.99                     | 0.40              |
| 22:c:6033:CLA:H3A  | 22:c:6033:CLA:HBA1 | 1.75                     | 0.40              |
| 22:c:6035:CLA:HAA1 | 22:c:6035:CLA:CBD  | 2.52                     | 0.40              |
| 4:d:5046:GLY:HA2   | 25:d:6050:BCR:H10C | 2.02                     | 0.40              |
| 4:d:5087:HIS:C     | 4:d:5167:TRP:NE1   | 2.78                     | 0.40              |
| 4:d:5153:PHE:O     | 4:d:5157:PHE:HB2   | 2.20                     | 0.40              |
| 7:h:5006:TRP:CD1   | 7:h:5010:ILE:CD1   | 2.88                     | 0.40              |
| 7:h:5046:LEU:HD23  | 7:h:5046:LEU:C     | 2.46                     | 0.40              |
| 7:h:5047:GLU:OE2   | 7:h:5052:THR:HG21  | 2.21                     | 0.40              |
| 8:i:5011:VAL:O     | 8:i:5015:PHE:HD1   | 2.04                     | 0.40              |
| 9:j:5035:GLY:O     | 9:j:5036:LEU:C     | 2.62                     | 0.40              |
| 20:z:5012:LEU:CD2  | 20:z:5054:VAL:HG21 | 2.52                     | 0.40              |
| 25:z:6053:BCR:H403 | 25:z:6053:BCR:H24C | 1.86                     | 0.40              |
| 1:A:150:PRO:C      | 22:A:1003:CLA:H52  | 2.46                     | 0.40              |
| 1:A:153:SER:O      | 1:A:156:ALA:N      | 2.55                     | 0.40              |
| 1:A:277:ALA:O      | 1:A:278:TRP:C      | 2.64                     | 0.40              |
| 1:A:316:THR:CG2    | 4:D:75:THR:HG23    | 2.51                     | 0.40              |
| 1:A:318:ALA:O      | 1:A:321:ILE:HB     | 2.21                     | 0.40              |
| 2:B:149:LEU:HD13   | 22:B:1012:CLA:H203 | 2.03                     | 0.40              |
| 2:B:158:LEU:C      | 2:B:160:GLY:H      | 2.28                     | 0.40              |
| 2:B:208:VAL:HG21   | 22:B:1010:CLA:HMC2 | 2.02                     | 0.40              |
| 2:B:468:TRP:CZ2    | 22:B:1019:CLA:HED2 | 2.56                     | 0.40              |
| 22:B:1022:CLA:H143 | 22:B:1022:CLA:H71  | 1.94                     | 0.40              |
| 22:B:1022:CLA:OBD  | 11:L:10:VAL:HG21   | 2.20                     | 0.40              |
| 22:B:1023:CLA:C4D  | 22:B:1024:CLA:CMC  | 2.99                     | 0.40              |
| 3:C:257:PHE:O      | 3:C:261:ARG:HG3    | 2.21                     | 0.40              |
| 4:D:111:TRP:CE2    | 4:D:173:PHE:HE2    | 2.38                     | 0.40              |
| 4:D:171:PRO:HA     | 4:D:181:PHE:CE2    | 2.55                     | 0.40              |
| 4:D:176:ALA:C      | 4:D:178:ILE:N      | 2.79                     | 0.40              |
| 5:E:8:ARG:HH21     | 6:F:13:TYR:H       | 1.68                     | 0.40              |
| 9:J:21:VAL:HG12    | 9:J:22:ILE:CD1     | 2.35                     | 0.40              |
| 9:J:34:ALA:O       | 9:J:35:GLY:C       | 2.64                     | 0.40              |
| 22:K:1034:CLA:H162 | 22:K:1034:CLA:H141 | 1.70                     | 0.40              |
| 28:L:1061:MGE:H7B1 | 28:L:1061:MGE:C3B  | 2.51                     | 0.40              |
| 12:M:9:ILE:CD1     | 12:m:5008:PHE:HB3  | 2.51                     | 0.40              |
| 13:O:223:ILE:HD13  | 13:O:225:LEU:CD1   | 2.50                     | 0.40              |
| 15:U:9:LEU:H       | 15:U:9:LEU:HG      | 1.47                     | 0.40              |
| 17:X:43:ILE:O      | 17:X:44:ASP:HB2    | 2.22                     | 0.40              |
| 1:a:5099:ALA:O     | 1:a:5100:ALA:O     | 2.38                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5187:GLN:HE22  | 1:a:5193:LEU:HB2   | 1.87                     | 0.40              |
| 22:a:6007:CLA:H142 | 22:a:6007:CLA:H111 | 1.67                     | 0.40              |
| 2:b:5093:PHE:O     | 2:b:5094:GLU:C     | 2.64                     | 0.40              |
| 2:b:5275:TRP:CH2   | 2:b:5358:ARG:HD3   | 2.56                     | 0.40              |
| 2:b:5394:GLN:HB3   | 15:u:5017:LEU:HD22 | 2.02                     | 0.40              |
| 3:c:5063:TRP:CH2   | 22:c:6026:CLA:HMB3 | 2.56                     | 0.40              |
| 3:c:5110:PRO:O     | 3:c:5113:VAL:HB    | 2.21                     | 0.40              |
| 3:c:5362:ARG:NH1   | 3:c:5362:ARG:HG3   | 2.37                     | 0.40              |
| 3:c:5449:ARG:O     | 3:c:5452:ALA:HB3   | 2.22                     | 0.40              |
| 4:d:5100:ASP:O     | 4:d:5103:ARG:N     | 2.54                     | 0.40              |
| 4:d:5221:THR:O     | 4:d:5244:TYR:CA    | 2.64                     | 0.40              |
| 4:d:5313:THR:H     | 4:d:5316:THR:CG2   | 2.34                     | 0.40              |
| 7:h:5019:GLY:O     | 7:h:5020:LYS:C     | 2.65                     | 0.40              |
| 7:h:5053:LEU:CD1   | 7:h:5055:LEU:HD21  | 2.44                     | 0.40              |
| 9:j:5024:ILE:O     | 9:j:5027:LEU:HB3   | 2.22                     | 0.40              |
| 9:j:5034:ALA:O     | 9:j:5035:GLY:O     | 2.39                     | 0.40              |
| 10:k:5011:LEU:O    | 10:k:5012:PRO:C    | 2.63                     | 0.40              |
| 10:k:5017:ILE:H    | 10:k:5017:ILE:HG13 | 1.47                     | 0.40              |
| 12:m:5028:GLN:HG3  | 12:m:5029:THR:N    | 2.36                     | 0.40              |
| 13:o:5166:THR:HG22 | 13:o:5167:ASP:N    | 2.36                     | 0.40              |
| 13:o:5195:ASP:O    | 13:o:5195:ASP:CG   | 2.65                     | 0.40              |
| 15:u:5036:ILE:HG13 | 15:u:5037:GLN:N    | 2.36                     | 0.40              |
| 1:A:105:TRP:HZ3    | 25:A:1044:BCR:C39  | 2.33                     | 0.40              |
| 1:A:133:LEU:HB3    | 4:D:252:PHE:CE2    | 2.57                     | 0.40              |
| 1:A:147:TYR:HA     | 23:A:1038:PHO:HMD2 | 2.03                     | 0.40              |
| 1:A:213:ALA:HB3    | 23:D:1039:PHO:CBC  | 2.50                     | 0.40              |
| 1:A:259:ILE:O      | 1:A:260:PHE:HB2    | 2.20                     | 0.40              |
| 2:B:18:ARG:HH11    | 11:L:4:ASN:ND2     | 2.19                     | 0.40              |
| 2:B:103:LEU:HD22   | 22:B:1014:CLA:H61  | 2.04                     | 0.40              |
| 2:B:113:TRP:CD1    | 2:B:113:TRP:C      | 2.98                     | 0.40              |
| 2:B:115:TRP:HB2    | 27:B:1067:IOD:I    | 2.91                     | 0.40              |
| 2:B:174:LEU:HD21   | 2:B:265:ILE:HB     | 2.04                     | 0.40              |
| 2:B:237:VAL:HG12   | 22:B:1020:CLA:HMD1 | 2.03                     | 0.40              |
| 3:C:282:MET:HE2    | 3:C:282:MET:HB2    | 1.84                     | 0.40              |
| 3:C:305:THR:O      | 3:C:305:THR:HG23   | 2.21                     | 0.40              |
| 3:C:322:GLN:HB2    | 3:C:328:VAL:HG21   | 2.03                     | 0.40              |
| 3:C:362:ARG:NH1    | 3:C:362:ARG:HG3    | 2.37                     | 0.40              |
| 22:C:1029:CLA:C1C  | 22:C:1029:CLA:H41  | 2.52                     | 0.40              |
| 22:C:1031:CLA:HAA2 | 22:C:1031:CLA:CB D | 2.51                     | 0.40              |
| 22:C:1031:CLA:CMD  | 22:C:1033:CLA:C16  | 2.99                     | 0.40              |
| 22:C:1032:CLA:HBC2 | 22:C:1032:CLA:CHD  | 2.47                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:54:PHE:HD1     | 5:E:47:PHE:HE1     | 1.68                     | 0.40              |
| 4:D:103:ARG:HG3    | 4:D:103:ARG:HH11   | 1.87                     | 0.40              |
| 4:D:103:ARG:HA     | 4:D:106:GLN:HB2    | 2.04                     | 0.40              |
| 5:E:49:THR:HA      | 5:E:50:PRO:HD3     | 1.88                     | 0.40              |
| 8:I:6:ILE:O        | 8:I:10:ILE:CD1     | 2.70                     | 0.40              |
| 8:I:11:VAL:O       | 8:I:15:PHE:HD1     | 2.04                     | 0.40              |
| 9:J:24:ILE:O       | 9:J:27:LEU:HB3     | 2.21                     | 0.40              |
| 16:V:47:LEU:HD23   | 16:V:48:THR:O      | 2.21                     | 0.40              |
| 31:V:1041:HEM:HHC  | 31:V:1041:HEM:CBB  | 2.51                     | 0.40              |
| 1:a:5143:ILE:CB    | 4:d:5220:ASN:ND2   | 2.78                     | 0.40              |
| 23:a:6038:PHO:H93  | 23:a:6038:PHO:H62  | 1.68                     | 0.40              |
| 2:b:5003:LEU:N     | 11:l:5011:GLU:HB2  | 2.36                     | 0.40              |
| 2:b:5030:VAL:HG12  | 2:b:5031:ALA:N     | 2.37                     | 0.40              |
| 2:b:5065:PHE:O     | 2:b:5066:MET:C     | 2.63                     | 0.40              |
| 2:b:5069:LEU:HD12  | 2:b:5069:LEU:HA    | 1.84                     | 0.40              |
| 2:b:5149:LEU:HD13  | 22:b:6012:CLA:H203 | 2.03                     | 0.40              |
| 2:b:5206:GLY:O     | 2:b:5210:ILE:HG13  | 2.21                     | 0.40              |
| 3:c:5080:PRO:HB2   | 3:c:5083:GLU:HG3   | 2.03                     | 0.40              |
| 3:c:5157:MET:CE    | 3:c:5271:TYR:CD2   | 3.05                     | 0.40              |
| 3:c:5205:ASP:HA    | 3:c:5206:PRO:HD2   | 2.00                     | 0.40              |
| 3:c:5321:ASP:HB2   | 3:c:5340:TYR:CE1   | 2.56                     | 0.40              |
| 3:c:5348:GLU:CB    | 13:o:5042:ALA:CB   | 2.84                     | 0.40              |
| 22:c:6027:CLA:H143 | 22:c:6027:CLA:H112 | 1.87                     | 0.40              |
| 22:c:6028:CLA:C1C  | 29:c:6056:DGD:HA31 | 2.47                     | 0.40              |
| 29:c:6056:DGD:HG12 | 29:c:6056:DGD:HB21 | 2.02                     | 0.40              |
| 4:d:5090:LEU:HD23  | 4:d:5109:GLY:HA2   | 2.04                     | 0.40              |
| 4:d:5103:ARG:HG3   | 4:d:5103:ARG:HH11  | 1.87                     | 0.40              |
| 4:d:5305:ALA:CB    | 13:o:5186:LYS:HD2  | 2.47                     | 0.40              |
| 4:d:5352:LEU:HB2   | 16:v:5160:LYS:HE2  | 2.04                     | 0.40              |
| 23:d:6039:PHO:H92  | 23:d:6039:PHO:H111 | 1.74                     | 0.40              |
| 23:d:6039:PHO:HAA2 | 23:d:6039:PHO:HBD  | 2.03                     | 0.40              |
| 8:i:5006:ILE:O     | 8:i:5010:ILE:CD1   | 2.70                     | 0.40              |
| 11:l:5027:LEU:O    | 11:l:5028:ALA:C    | 2.65                     | 0.40              |
| 13:o:5118:SER:HB3  | 13:o:5157:PRO:HA   | 2.03                     | 0.40              |
| 13:o:5265:PHE:HD1  | 13:o:5266:TYR:O    | 2.04                     | 0.40              |
| 14:t:5012:CYS:CA   | 27:t:6066:IOD:I    | 3.39                     | 0.40              |
| 14:t:5014:ILE:CG2  | 14:t:5015:ALA:N    | 2.84                     | 0.40              |
| 1:A:38:ILE:HB      | 1:A:39:PRO:HD3     | 2.02                     | 0.40              |
| 1:A:49:VAL:HG23    | 1:A:50:ILE:HG13    | 2.04                     | 0.40              |
| 1:A:55:ALA:O       | 1:A:73:TYR:CD2     | 2.74                     | 0.40              |
| 1:A:173:PRO:HG2    | 1:A:178:GLY:HA3    | 2.04                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:187:GLN:CG     | 1:A:328:MET:HE1    | 2.51                     | 0.40              |
| 1:A:224:ILE:C      | 2:B:482:ILE:H      | 2.30                     | 0.40              |
| 1:A:331:MET:HE1    | 4:D:348:ARG:C      | 2.47                     | 0.40              |
| 2:B:23:HIS:CD2     | 22:B:1020:CLA:HBA2 | 2.57                     | 0.40              |
| 2:B:206:GLY:O      | 2:B:210:ILE:HG13   | 2.21                     | 0.40              |
| 3:C:42:LEU:HD22    | 22:C:1035:CLA:CMA  | 2.52                     | 0.40              |
| 3:C:171:GLY:C      | 3:C:174:LEU:N      | 2.79                     | 0.40              |
| 3:C:188:THR:CG2    | 3:C:300:GLU:OE1    | 2.69                     | 0.40              |
| 3:C:222:GLY:HA3    | 3:C:225:VAL:HG22   | 2.03                     | 0.40              |
| 3:C:284:PHE:CB     | 29:C:1055:DGD:HB71 | 2.44                     | 0.40              |
| 3:C:459:ILE:O      | 4:D:223:PHE:HA     | 2.21                     | 0.40              |
| 22:C:1028:CLA:H62  | 22:C:1028:CLA:H41  | 1.42                     | 0.40              |
| 22:C:1029:CLA:CMD  | 22:C:1031:CLA:CBB  | 2.99                     | 0.40              |
| 4:D:66:SER:N       | 4:D:71:CYS:SG      | 2.94                     | 0.40              |
| 24:D:1042:PQ9:H361 | 24:D:1042:PQ9:H32  | 1.77                     | 0.40              |
| 7:H:2:ALA:O        | 7:H:3:ARG:HB2      | 2.21                     | 0.40              |
| 7:H:19:GLY:O       | 7:H:20:LYS:C       | 2.65                     | 0.40              |
| 9:J:15:THR:CG2     | 10:K:38:VAL:HG22   | 2.51                     | 0.40              |
| 13:O:187:GLY:O     | 13:O:194:TYR:N     | 2.51                     | 0.40              |
| 15:U:68:THR:HG23   | 15:U:71:GLN:H      | 1.80                     | 0.40              |
| 16:V:62:ALA:O      | 31:V:1041:HEM:CBB  | 2.68                     | 0.40              |
| 20:Z:48:ILE:O      | 20:Z:52:LEU:HD12   | 2.22                     | 0.40              |
| 1:a:5076:ASN:ND2   | 11:l:5033:SER:C    | 2.80                     | 0.40              |
| 1:a:5147:TYR:HA    | 23:a:6038:PHO:HMD2 | 2.03                     | 0.40              |
| 1:a:5183:MET:O     | 1:a:5184:ILE:C     | 2.65                     | 0.40              |
| 1:a:5228:THR:CG2   | 1:a:5230:THR:HG23  | 2.52                     | 0.40              |
| 1:a:5233:ALA:C     | 4:d:5265:ARG:HH12  | 2.29                     | 0.40              |
| 1:a:5291:SER:O     | 1:a:5294:ALA:HB3   | 2.22                     | 0.40              |
| 22:a:6006:CLA:HMB2 | 23:d:6039:PHO:H152 | 2.04                     | 0.40              |
| 2:b:5033:TRP:HH2   | 2:b:5062:VAL:CG2   | 2.34                     | 0.40              |
| 2:b:5102:VAL:O     | 2:b:5106:LEU:HG    | 2.22                     | 0.40              |
| 2:b:5135:LEU:H     | 2:b:5136:PRO:CD    | 2.35                     | 0.40              |
| 2:b:5221:PRO:HA    | 2:b:5222:PRO:HD3   | 1.98                     | 0.40              |
| 2:b:5223:GLN:HG2   | 7:h:5021:VAL:CG2   | 2.52                     | 0.40              |
| 2:b:5269:GLY:O     | 2:b:5448:ARG:NH1   | 2.55                     | 0.40              |
| 22:b:6010:CLA:H41  | 22:b:6010:CLA:H61  | 1.84                     | 0.40              |
| 22:b:6023:CLA:C4D  | 22:b:6024:CLA:CMC  | 2.99                     | 0.40              |
| 22:b:6024:CLA:HAA2 | 22:b:6024:CLA:CBD  | 2.51                     | 0.40              |
| 28:b:6060:MGE:H7B1 | 28:b:6060:MGE:H3B1 | 1.95                     | 0.40              |
| 3:c:5041:ARG:NH2   | 22:c:6035:CLA:HMD2 | 2.37                     | 0.40              |
| 3:c:5356:MET:O     | 3:c:5358:PHE:N     | 2.55                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:c:5406:SER:CB    | 29:c:6056:DGD:HE1 | 2.39                     | 0.40              |
| 4:d:5066:SER:N     | 4:d:5071:CYS:SG   | 2.94                     | 0.40              |
| 4:d:5100:ASP:C     | 4:d:5102:THR:N    | 2.80                     | 0.40              |
| 28:d:6062:MGE:O1B  | 28:d:6062:MGE:O1G | 2.39                     | 0.40              |
| 13:o:5099:ARG:HH11 | 13:o:5099:ARG:CG  | 2.34                     | 0.40              |
| 13:o:5144:LEU:HD23 | 13:o:5144:LEU:N   | 2.31                     | 0.40              |
| 13:o:5188:ARG:HD3  | 13:o:5212:ASN:OD1 | 2.21                     | 0.40              |
| 13:o:5214:LYS:CE   | 13:o:5251:MET:HG3 | 2.39                     | 0.40              |
| 15:u:5088:GLU:O    | 15:u:5089:THR:C   | 2.65                     | 0.40              |
| 16:v:5094:ASN:O    | 16:v:5096:GLU:N   | 2.55                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 1   | A     | 333/344 (97%)  | 219 (66%) | 75 (22%) | 39 (12%) | 0           | 5  |
| 1   | a     | 333/344 (97%)  | 216 (65%) | 76 (23%) | 41 (12%) | 0           | 4  |
| 2   | B     | 486/488 (100%) | 350 (72%) | 86 (18%) | 50 (10%) | 0           | 7  |
| 2   | b     | 486/488 (100%) | 350 (72%) | 86 (18%) | 50 (10%) | 0           | 7  |
| 3   | C     | 445/447 (100%) | 330 (74%) | 80 (18%) | 35 (8%)  | 1           | 12 |
| 3   | c     | 445/447 (100%) | 330 (74%) | 80 (18%) | 35 (8%)  | 1           | 12 |
| 4   | D     | 338/340 (99%)  | 222 (66%) | 78 (23%) | 38 (11%) | 0           | 6  |
| 4   | d     | 338/340 (99%)  | 224 (66%) | 77 (23%) | 37 (11%) | 0           | 7  |
| 5   | E     | 80/83 (96%)    | 54 (68%)  | 17 (21%) | 9 (11%)  | 0           | 5  |
| 5   | e     | 80/83 (96%)    | 54 (68%)  | 17 (21%) | 9 (11%)  | 0           | 5  |
| 6   | F     | 33/44 (75%)    | 20 (61%)  | 9 (27%)  | 4 (12%)  | 0           | 4  |
| 6   | f     | 33/44 (75%)    | 20 (61%)  | 9 (27%)  | 4 (12%)  | 0           | 4  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-----------|-------------|-----|
| 7   | H     | 62/64 (97%)     | 42 (68%)   | 12 (19%)  | 8 (13%)   | 0           | 4   |
| 7   | h     | 62/64 (97%)     | 42 (68%)   | 12 (19%)  | 8 (13%)   | 0           | 4   |
| 8   | I     | 33/35 (94%)     | 21 (64%)   | 6 (18%)   | 6 (18%)   | 0           | 2   |
| 8   | i     | 33/35 (94%)     | 21 (64%)   | 6 (18%)   | 6 (18%)   | 0           | 2   |
| 9   | J     | 32/40 (80%)     | 29 (91%)   | 0         | 3 (9%)    | 0           | 10  |
| 9   | j     | 32/40 (80%)     | 29 (91%)   | 0         | 3 (9%)    | 0           | 10  |
| 10  | K     | 34/36 (94%)     | 23 (68%)   | 5 (15%)   | 6 (18%)   | 0           | 2   |
| 10  | k     | 34/36 (94%)     | 17 (50%)   | 8 (24%)   | 9 (26%)   | 0           | 0   |
| 11  | L     | 35/37 (95%)     | 25 (71%)   | 8 (23%)   | 2 (6%)    | 1           | 17  |
| 11  | l     | 35/37 (95%)     | 25 (71%)   | 8 (23%)   | 2 (6%)    | 1           | 17  |
| 12  | M     | 34/36 (94%)     | 23 (68%)   | 11 (32%)  | 0         | 100         | 100 |
| 12  | m     | 34/36 (94%)     | 23 (68%)   | 11 (32%)  | 0         | 100         | 100 |
| 13  | O     | 240/242 (99%)   | 172 (72%)  | 41 (17%)  | 27 (11%)  | 0           | 5   |
| 13  | o     | 240/242 (99%)   | 172 (72%)  | 41 (17%)  | 27 (11%)  | 0           | 5   |
| 14  | T     | 28/30 (93%)     | 22 (79%)   | 5 (18%)   | 1 (4%)    | 2           | 23  |
| 14  | t     | 28/30 (93%)     | 22 (79%)   | 4 (14%)   | 2 (7%)    | 1           | 14  |
| 15  | U     | 96/98 (98%)     | 70 (73%)   | 17 (18%)  | 9 (9%)    | 0           | 10  |
| 15  | u     | 96/98 (98%)     | 70 (73%)   | 18 (19%)  | 8 (8%)    | 0           | 11  |
| 16  | V     | 135/137 (98%)   | 100 (74%)  | 25 (18%)  | 10 (7%)   | 1           | 13  |
| 16  | v     | 135/137 (98%)   | 99 (73%)   | 26 (19%)  | 10 (7%)   | 1           | 13  |
| 17  | X     | 32/34 (94%)     | 29 (91%)   | 3 (9%)    | 0         | 100         | 100 |
| 17  | x     | 32/34 (94%)     | 29 (91%)   | 3 (9%)    | 0         | 100         | 100 |
| 18  | Y     | 26/28 (93%)     | 20 (77%)   | 1 (4%)    | 5 (19%)   | 0           | 2   |
| 18  | y     | 26/28 (93%)     | 20 (77%)   | 1 (4%)    | 5 (19%)   | 0           | 2   |
| 20  | Z     | 60/62 (97%)     | 44 (73%)   | 12 (20%)  | 4 (7%)    | 1           | 15  |
| 20  | z     | 60/62 (97%)     | 44 (73%)   | 12 (20%)  | 4 (7%)    | 1           | 15  |
| All | All   | 5124/5250 (98%) | 3622 (71%) | 986 (19%) | 516 (10%) | 0           | 8   |

All (516) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 60  | ILE  |
| 1   | A     | 61  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 100 | ALA  |
| 1   | A     | 224 | ILE  |
| 1   | A     | 226 | GLU  |
| 1   | A     | 337 | HIS  |
| 2   | B     | 11  | VAL  |
| 2   | B     | 36  | SER  |
| 2   | B     | 48  | SER  |
| 2   | B     | 93  | PHE  |
| 2   | B     | 112 | CYS  |
| 2   | B     | 171 | PRO  |
| 2   | B     | 230 | ARG  |
| 2   | B     | 250 | PHE  |
| 2   | B     | 278 | SER  |
| 2   | B     | 322 | GLY  |
| 2   | B     | 327 | THR  |
| 2   | B     | 330 | MET  |
| 2   | B     | 361 | ALA  |
| 2   | B     | 407 | ASN  |
| 2   | B     | 484 | PRO  |
| 2   | B     | 487 | SER  |
| 3   | C     | 85  | GLY  |
| 3   | C     | 132 | HIS  |
| 3   | C     | 144 | SER  |
| 3   | C     | 146 | PHE  |
| 3   | C     | 150 | ASP  |
| 3   | C     | 191 | PRO  |
| 3   | C     | 274 | TYR  |
| 3   | C     | 275 | SER  |
| 3   | C     | 416 | SER  |
| 3   | C     | 452 | ALA  |
| 4   | D     | 21  | TRP  |
| 4   | D     | 25  | ASP  |
| 4   | D     | 80  | THR  |
| 4   | D     | 101 | PHE  |
| 4   | D     | 109 | GLY  |
| 4   | D     | 110 | LEU  |
| 4   | D     | 171 | PRO  |
| 4   | D     | 263 | ASN  |
| 4   | D     | 276 | VAL  |
| 4   | D     | 297 | ASP  |
| 4   | D     | 300 | SER  |
| 4   | D     | 351 | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | F     | 23   | VAL  |
| 6   | F     | 41   | GLN  |
| 6   | F     | 43   | ILE  |
| 7   | H     | 18   | TYR  |
| 7   | H     | 64   | ALA  |
| 8   | I     | 26   | GLY  |
| 8   | I     | 34   | ARG  |
| 9   | J     | 39   | SER  |
| 11  | L     | 6    | ASN  |
| 13  | O     | 46   | PRO  |
| 13  | O     | 60   | SER  |
| 13  | O     | 88   | GLU  |
| 13  | O     | 115  | SER  |
| 13  | O     | 166  | THR  |
| 13  | O     | 182  | PHE  |
| 13  | O     | 207  | GLU  |
| 13  | O     | 253  | ALA  |
| 15  | U     | 37   | GLN  |
| 15  | U     | 42   | TYR  |
| 15  | U     | 43   | PRO  |
| 15  | U     | 53   | ALA  |
| 16  | V     | 160  | LYS  |
| 18  | Y     | 20   | ALA  |
| 18  | Y     | 21   | GLN  |
| 18  | Y     | 43   | ARG  |
| 18  | Y     | 44   | GLY  |
| 1   | a     | 5060 | ILE  |
| 1   | a     | 5061 | ASP  |
| 1   | a     | 5100 | ALA  |
| 1   | a     | 5224 | ILE  |
| 1   | a     | 5226 | GLU  |
| 1   | a     | 5337 | HIS  |
| 2   | b     | 5011 | VAL  |
| 2   | b     | 5036 | SER  |
| 2   | b     | 5048 | SER  |
| 2   | b     | 5093 | PHE  |
| 2   | b     | 5112 | CYS  |
| 2   | b     | 5171 | PRO  |
| 2   | b     | 5230 | ARG  |
| 2   | b     | 5250 | PHE  |
| 2   | b     | 5278 | SER  |
| 2   | b     | 5322 | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | b     | 5327 | THR  |
| 2   | b     | 5330 | MET  |
| 2   | b     | 5361 | ALA  |
| 2   | b     | 5407 | ASN  |
| 2   | b     | 5484 | PRO  |
| 2   | b     | 5487 | SER  |
| 3   | c     | 5085 | GLY  |
| 3   | c     | 5132 | HIS  |
| 3   | c     | 5144 | SER  |
| 3   | c     | 5146 | PHE  |
| 3   | c     | 5150 | ASP  |
| 3   | c     | 5191 | PRO  |
| 3   | c     | 5274 | TYR  |
| 3   | c     | 5275 | SER  |
| 3   | c     | 5416 | SER  |
| 3   | c     | 5452 | ALA  |
| 4   | d     | 5021 | TRP  |
| 4   | d     | 5025 | ASP  |
| 4   | d     | 5080 | THR  |
| 4   | d     | 5101 | PHE  |
| 4   | d     | 5109 | GLY  |
| 4   | d     | 5110 | LEU  |
| 4   | d     | 5171 | PRO  |
| 4   | d     | 5263 | ASN  |
| 4   | d     | 5276 | VAL  |
| 4   | d     | 5297 | ASP  |
| 4   | d     | 5300 | SER  |
| 4   | d     | 5351 | ALA  |
| 6   | f     | 5023 | VAL  |
| 6   | f     | 5041 | GLN  |
| 6   | f     | 5043 | ILE  |
| 7   | h     | 5018 | TYR  |
| 7   | h     | 5064 | ALA  |
| 8   | i     | 5026 | GLY  |
| 8   | i     | 5034 | ARG  |
| 9   | j     | 5039 | SER  |
| 10  | k     | 5032 | PHE  |
| 10  | k     | 5034 | ALA  |
| 11  | l     | 5006 | ASN  |
| 13  | o     | 5046 | PRO  |
| 13  | o     | 5060 | SER  |
| 13  | o     | 5088 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 13  | o     | 5115 | SER  |
| 13  | o     | 5166 | THR  |
| 13  | o     | 5182 | PHE  |
| 13  | o     | 5207 | GLU  |
| 13  | o     | 5253 | ALA  |
| 15  | u     | 5037 | GLN  |
| 15  | u     | 5042 | TYR  |
| 15  | u     | 5043 | PRO  |
| 15  | u     | 5053 | ALA  |
| 16  | v     | 5160 | LYS  |
| 18  | y     | 5020 | ALA  |
| 18  | y     | 5021 | GLN  |
| 18  | y     | 5043 | ARG  |
| 18  | y     | 5044 | GLY  |
| 1   | A     | 27   | ARG  |
| 1   | A     | 49   | VAL  |
| 1   | A     | 122  | GLY  |
| 1   | A     | 141  | PRO  |
| 1   | A     | 258  | LEU  |
| 1   | A     | 309  | ALA  |
| 1   | A     | 310  | LYS  |
| 1   | A     | 334  | ARG  |
| 2   | B     | 12   | LEU  |
| 2   | B     | 13   | ILE  |
| 2   | B     | 56   | TRP  |
| 2   | B     | 58   | GLN  |
| 2   | B     | 103  | LEU  |
| 2   | B     | 114  | HIS  |
| 2   | B     | 126  | PRO  |
| 2   | B     | 165  | GLY  |
| 2   | B     | 307  | GLU  |
| 2   | B     | 321  | LYS  |
| 2   | B     | 358  | ARG  |
| 2   | B     | 373  | LYS  |
| 2   | B     | 415  | PRO  |
| 3   | C     | 145  | SER  |
| 3   | C     | 153  | ASP  |
| 3   | C     | 192  | GLY  |
| 3   | C     | 310  | SER  |
| 3   | C     | 398  | HIS  |
| 4   | D     | 34   | GLY  |
| 4   | D     | 79   | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 141  | TYR  |
| 4   | D     | 182  | LEU  |
| 4   | D     | 275  | PRO  |
| 4   | D     | 307  | GLU  |
| 4   | D     | 327  | ALA  |
| 5   | E     | 57   | ALA  |
| 5   | E     | 60   | GLN  |
| 5   | E     | 78   | THR  |
| 5   | E     | 81   | GLU  |
| 7   | H     | 3    | ARG  |
| 7   | H     | 51   | SER  |
| 8   | I     | 25   | SER  |
| 8   | I     | 30   | ARG  |
| 9   | J     | 31   | GLY  |
| 10  | K     | 31   | LEU  |
| 10  | K     | 44   | GLY  |
| 11  | L     | 14   | ARG  |
| 13  | O     | 50   | ASP  |
| 13  | O     | 64   | TYR  |
| 13  | O     | 138  | GLY  |
| 13  | O     | 164  | THR  |
| 13  | O     | 175  | PRO  |
| 13  | O     | 179  | THR  |
| 13  | O     | 194  | TYR  |
| 13  | O     | 198  | ILE  |
| 13  | O     | 222  | GLN  |
| 13  | O     | 267  | ALA  |
| 15  | U     | 30   | THR  |
| 15  | U     | 52   | ASN  |
| 15  | U     | 60   | ASP  |
| 15  | U     | 79   | LEU  |
| 16  | V     | 59   | PHE  |
| 16  | V     | 63   | CYS  |
| 16  | V     | 97   | GLY  |
| 20  | Z     | 44   | SER  |
| 20  | Z     | 55   | GLY  |
| 1   | a     | 5027 | ARG  |
| 1   | a     | 5049 | VAL  |
| 1   | a     | 5122 | GLY  |
| 1   | a     | 5141 | PRO  |
| 1   | a     | 5258 | LEU  |
| 1   | a     | 5309 | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 5310 | LYS  |
| 1   | a     | 5334 | ARG  |
| 1   | a     | 5336 | ALA  |
| 2   | b     | 5012 | LEU  |
| 2   | b     | 5013 | ILE  |
| 2   | b     | 5056 | TRP  |
| 2   | b     | 5058 | GLN  |
| 2   | b     | 5103 | LEU  |
| 2   | b     | 5114 | HIS  |
| 2   | b     | 5126 | PRO  |
| 2   | b     | 5165 | GLY  |
| 2   | b     | 5307 | GLU  |
| 2   | b     | 5321 | LYS  |
| 2   | b     | 5358 | ARG  |
| 2   | b     | 5373 | LYS  |
| 2   | b     | 5415 | PRO  |
| 3   | c     | 5145 | SER  |
| 3   | c     | 5153 | ASP  |
| 3   | c     | 5192 | GLY  |
| 3   | c     | 5310 | SER  |
| 3   | c     | 5398 | HIS  |
| 4   | d     | 5034 | GLY  |
| 4   | d     | 5079 | SER  |
| 4   | d     | 5141 | TYR  |
| 4   | d     | 5182 | LEU  |
| 4   | d     | 5275 | PRO  |
| 4   | d     | 5307 | GLU  |
| 4   | d     | 5327 | ALA  |
| 5   | e     | 5057 | ALA  |
| 5   | e     | 5060 | GLN  |
| 5   | e     | 5078 | THR  |
| 5   | e     | 5081 | GLU  |
| 7   | h     | 5003 | ARG  |
| 7   | h     | 5051 | SER  |
| 8   | i     | 5025 | SER  |
| 8   | i     | 5030 | ARG  |
| 9   | j     | 5031 | GLY  |
| 10  | k     | 5033 | PHE  |
| 10  | k     | 5044 | GLY  |
| 11  | l     | 5014 | ARG  |
| 13  | o     | 5050 | ASP  |
| 13  | o     | 5064 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 13  | o     | 5138 | GLY  |
| 13  | o     | 5164 | THR  |
| 13  | o     | 5175 | PRO  |
| 13  | o     | 5179 | THR  |
| 13  | o     | 5194 | TYR  |
| 13  | o     | 5198 | ILE  |
| 13  | o     | 5222 | GLN  |
| 13  | o     | 5267 | ALA  |
| 14  | t     | 5012 | CYS  |
| 15  | u     | 5030 | THR  |
| 15  | u     | 5052 | ASN  |
| 15  | u     | 5060 | ASP  |
| 15  | u     | 5079 | LEU  |
| 16  | v     | 5059 | PHE  |
| 16  | v     | 5063 | CYS  |
| 16  | v     | 5097 | GLY  |
| 20  | z     | 5044 | SER  |
| 20  | z     | 5055 | GLY  |
| 1   | A     | 35   | VAL  |
| 1   | A     | 48   | PHE  |
| 1   | A     | 108  | ASN  |
| 1   | A     | 120  | LEU  |
| 1   | A     | 260  | PHE  |
| 1   | A     | 298  | ASN  |
| 2   | B     | 75   | TRP  |
| 2   | B     | 111  | ALA  |
| 2   | B     | 146  | ALA  |
| 2   | B     | 249  | ALA  |
| 2   | B     | 319  | PRO  |
| 2   | B     | 483  | ASP  |
| 3   | C     | 29   | GLU  |
| 3   | C     | 57   | ALA  |
| 3   | C     | 309  | ALA  |
| 3   | C     | 429  | SER  |
| 3   | C     | 430  | HIS  |
| 4   | D     | 19   | ASP  |
| 4   | D     | 22   | LEU  |
| 4   | D     | 111  | TRP  |
| 4   | D     | 183  | LEU  |
| 4   | D     | 192  | THR  |
| 4   | D     | 234  | ALA  |
| 4   | D     | 274  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 298  | PHE  |
| 4   | D     | 326  | ARG  |
| 5   | E     | 52   | PRO  |
| 5   | E     | 75   | GLN  |
| 5   | E     | 76   | VAL  |
| 5   | E     | 77   | GLU  |
| 7   | H     | 17   | GLU  |
| 7   | H     | 35   | MET  |
| 8   | I     | 2    | GLU  |
| 10  | K     | 16   | ALA  |
| 13  | O     | 53   | ARG  |
| 13  | O     | 68   | ARG  |
| 13  | O     | 252  | GLY  |
| 16  | V     | 107  | THR  |
| 16  | V     | 125  | ASP  |
| 16  | V     | 155  | LYS  |
| 20  | Z     | 22   | GLY  |
| 1   | a     | 5035 | VAL  |
| 1   | a     | 5048 | PHE  |
| 1   | a     | 5108 | ASN  |
| 1   | a     | 5120 | LEU  |
| 1   | a     | 5260 | PHE  |
| 1   | a     | 5298 | ASN  |
| 2   | b     | 5075 | TRP  |
| 2   | b     | 5111 | ALA  |
| 2   | b     | 5146 | ALA  |
| 2   | b     | 5249 | ALA  |
| 2   | b     | 5319 | PRO  |
| 2   | b     | 5483 | ASP  |
| 3   | c     | 5029 | GLU  |
| 3   | c     | 5057 | ALA  |
| 3   | c     | 5309 | ALA  |
| 3   | c     | 5429 | SER  |
| 3   | c     | 5430 | HIS  |
| 4   | d     | 5019 | ASP  |
| 4   | d     | 5022 | LEU  |
| 4   | d     | 5111 | TRP  |
| 4   | d     | 5183 | LEU  |
| 4   | d     | 5192 | THR  |
| 4   | d     | 5234 | ALA  |
| 4   | d     | 5274 | VAL  |
| 4   | d     | 5298 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | d     | 5326 | ARG  |
| 5   | e     | 5052 | PRO  |
| 5   | e     | 5075 | GLN  |
| 5   | e     | 5076 | VAL  |
| 5   | e     | 5077 | GLU  |
| 7   | h     | 5017 | GLU  |
| 7   | h     | 5035 | MET  |
| 8   | i     | 5002 | GLU  |
| 10  | k     | 5016 | ALA  |
| 10  | k     | 5031 | LEU  |
| 10  | k     | 5036 | ALA  |
| 13  | o     | 5053 | ARG  |
| 13  | o     | 5068 | ARG  |
| 13  | o     | 5252 | GLY  |
| 16  | v     | 5107 | THR  |
| 16  | v     | 5125 | ASP  |
| 16  | v     | 5155 | LYS  |
| 20  | z     | 5022 | GLY  |
| 1   | A     | 37   | MET  |
| 1   | A     | 81   | ALA  |
| 1   | A     | 150  | PRO  |
| 1   | A     | 172  | MET  |
| 1   | A     | 183  | MET  |
| 1   | A     | 268  | SER  |
| 1   | A     | 276  | ALA  |
| 2   | B     | 99   | ALA  |
| 2   | B     | 197  | GLY  |
| 2   | B     | 418  | LYS  |
| 3   | C     | 39   | ASN  |
| 3   | C     | 217  | PRO  |
| 3   | C     | 328  | VAL  |
| 3   | C     | 397  | THR  |
| 4   | D     | 20   | ASP  |
| 4   | D     | 27   | PHE  |
| 4   | D     | 90   | LEU  |
| 4   | D     | 113  | PHE  |
| 4   | D     | 268  | HIS  |
| 4   | D     | 299  | ILE  |
| 4   | D     | 343  | GLU  |
| 6   | F     | 14   | PRO  |
| 13  | O     | 212  | ASN  |
| 16  | V     | 47   | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 5037 | MET  |
| 1   | a     | 5081 | ALA  |
| 1   | a     | 5150 | PRO  |
| 1   | a     | 5172 | MET  |
| 1   | a     | 5183 | MET  |
| 1   | a     | 5268 | SER  |
| 1   | a     | 5276 | ALA  |
| 2   | b     | 5099 | ALA  |
| 2   | b     | 5197 | GLY  |
| 2   | b     | 5418 | LYS  |
| 3   | c     | 5039 | ASN  |
| 3   | c     | 5217 | PRO  |
| 3   | c     | 5328 | VAL  |
| 3   | c     | 5397 | THR  |
| 4   | d     | 5020 | ASP  |
| 4   | d     | 5027 | PHE  |
| 4   | d     | 5090 | LEU  |
| 4   | d     | 5113 | PHE  |
| 4   | d     | 5299 | ILE  |
| 4   | d     | 5343 | GLU  |
| 6   | f     | 5014 | PRO  |
| 13  | o     | 5212 | ASN  |
| 16  | v     | 5047 | LEU  |
| 1   | A     | 112  | TYR  |
| 1   | A     | 148  | SER  |
| 1   | A     | 237  | TYR  |
| 1   | A     | 259  | ILE  |
| 2   | B     | 100  | HIS  |
| 2   | B     | 231  | MET  |
| 2   | B     | 408  | GLY  |
| 2   | B     | 419  | SER  |
| 3   | C     | 306  | GLY  |
| 3   | C     | 472  | LEU  |
| 4   | D     | 251  | ARG  |
| 5   | E     | 48   | GLY  |
| 10  | K     | 36   | ALA  |
| 13  | O     | 143  | PRO  |
| 13  | O     | 192  | SER  |
| 14  | T     | 18   | PHE  |
| 18  | Y     | 45   | ASN  |
| 1   | a     | 5112 | TYR  |
| 1   | a     | 5148 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 5237 | TYR  |
| 1   | a     | 5259 | ILE  |
| 2   | b     | 5100 | HIS  |
| 2   | b     | 5231 | MET  |
| 2   | b     | 5419 | SER  |
| 3   | c     | 5306 | GLY  |
| 3   | c     | 5472 | LEU  |
| 4   | d     | 5251 | ARG  |
| 5   | e     | 5048 | GLY  |
| 7   | h     | 5028 | THR  |
| 13  | o     | 5143 | PRO  |
| 13  | o     | 5192 | SER  |
| 14  | t     | 5018 | PHE  |
| 18  | y     | 5045 | ASN  |
| 1   | A     | 38   | ILE  |
| 1   | A     | 39   | PRO  |
| 1   | A     | 63   | ILE  |
| 1   | A     | 227  | THR  |
| 1   | A     | 342  | ASP  |
| 2   | B     | 47   | PRO  |
| 2   | B     | 169  | SER  |
| 2   | B     | 186  | GLY  |
| 4   | D     | 292  | ASN  |
| 7   | H     | 28   | THR  |
| 8   | I     | 27   | ASP  |
| 13  | O     | 42   | ALA  |
| 13  | O     | 73   | PRO  |
| 13  | O     | 98   | THR  |
| 16  | V     | 71   | ILE  |
| 1   | a     | 5038 | ILE  |
| 1   | a     | 5039 | PRO  |
| 1   | a     | 5063 | ILE  |
| 1   | a     | 5227 | THR  |
| 1   | a     | 5342 | ASP  |
| 2   | b     | 5047 | PRO  |
| 2   | b     | 5169 | SER  |
| 2   | b     | 5408 | GLY  |
| 4   | d     | 5292 | ASN  |
| 8   | i     | 5027 | ASP  |
| 13  | o     | 5042 | ALA  |
| 13  | o     | 5073 | PRO  |
| 13  | o     | 5098 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | v     | 5071 | ILE  |
| 1   | A     | 90   | GLY  |
| 1   | A     | 184  | ILE  |
| 2   | B     | 234  | ILE  |
| 2   | B     | 414  | PRO  |
| 3   | C     | 183  | GLY  |
| 3   | C     | 233  | VAL  |
| 3   | C     | 380  | ILE  |
| 10  | K     | 25   | LEU  |
| 1   | a     | 5090 | GLY  |
| 1   | a     | 5184 | ILE  |
| 2   | b     | 5186 | GLY  |
| 2   | b     | 5234 | ILE  |
| 2   | b     | 5414 | PRO  |
| 3   | c     | 5183 | GLY  |
| 3   | c     | 5211 | GLY  |
| 3   | c     | 5233 | VAL  |
| 3   | c     | 5380 | ILE  |
| 10  | k     | 5025 | LEU  |
| 2   | B     | 191  | ASN  |
| 2   | B     | 219  | VAL  |
| 2   | B     | 264  | PRO  |
| 3   | C     | 101  | PRO  |
| 3   | C     | 102  | GLY  |
| 3   | C     | 208  | VAL  |
| 3   | C     | 211  | GLY  |
| 7   | H     | 40   | VAL  |
| 9   | J     | 35   | GLY  |
| 20  | Z     | 20   | VAL  |
| 2   | b     | 5191 | ASN  |
| 2   | b     | 5219 | VAL  |
| 2   | b     | 5264 | PRO  |
| 3   | c     | 5101 | PRO  |
| 3   | c     | 5102 | GLY  |
| 3   | c     | 5208 | VAL  |
| 7   | h     | 5040 | VAL  |
| 9   | j     | 5035 | GLY  |
| 20  | z     | 5020 | VAL  |
| 3   | C     | 205  | ASP  |
| 16  | V     | 76   | PRO  |
| 3   | c     | 5205 | ASP  |
| 16  | v     | 5076 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 195  | PRO  |
| 4   | d     | 5195 | PRO  |
| 1   | A     | 248  | ILE  |
| 3   | C     | 190  | ALA  |
| 10  | K     | 43   | VAL  |
| 15  | U     | 74   | ILE  |
| 1   | a     | 5236 | GLY  |
| 1   | a     | 5248 | ILE  |
| 3   | c     | 5190 | ALA  |
| 10  | k     | 5043 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 270/279 (97%)  | 213 (79%) | 57 (21%) | 1           | 7  |
| 1   | a     | 270/279 (97%)  | 213 (79%) | 57 (21%) | 1           | 7  |
| 2   | B     | 388/388 (100%) | 315 (81%) | 73 (19%) | 1           | 11 |
| 2   | b     | 388/388 (100%) | 315 (81%) | 73 (19%) | 1           | 11 |
| 3   | C     | 349/349 (100%) | 276 (79%) | 73 (21%) | 1           | 7  |
| 3   | c     | 349/349 (100%) | 276 (79%) | 73 (21%) | 1           | 7  |
| 4   | D     | 275/275 (100%) | 235 (86%) | 40 (14%) | 3           | 16 |
| 4   | d     | 275/275 (100%) | 235 (86%) | 40 (14%) | 3           | 16 |
| 5   | E     | 72/73 (99%)    | 57 (79%)  | 15 (21%) | 1           | 7  |
| 5   | e     | 72/73 (99%)    | 57 (79%)  | 15 (21%) | 1           | 7  |
| 6   | F     | 29/38 (76%)    | 22 (76%)  | 7 (24%)  | 1           | 5  |
| 6   | f     | 29/38 (76%)    | 22 (76%)  | 7 (24%)  | 1           | 5  |
| 7   | H     | 54/54 (100%)   | 45 (83%)  | 9 (17%)  | 2           | 13 |
| 7   | h     | 54/54 (100%)   | 45 (83%)  | 9 (17%)  | 2           | 13 |
| 8   | I     | 32/32 (100%)   | 24 (75%)  | 8 (25%)  | 0           | 4  |
| 8   | i     | 32/32 (100%)   | 24 (75%)  | 8 (25%)  | 0           | 4  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 9   | J     | 24/28 (86%)     | 18 (75%)   | 6 (25%)   | 0           | 4  |
| 9   | j     | 24/28 (86%)     | 18 (75%)   | 6 (25%)   | 0           | 4  |
| 10  | K     | 29/29 (100%)    | 21 (72%)   | 8 (28%)   | 0           | 3  |
| 10  | k     | 29/29 (100%)    | 23 (79%)   | 6 (21%)   | 1           | 7  |
| 11  | L     | 35/35 (100%)    | 29 (83%)   | 6 (17%)   | 2           | 13 |
| 11  | l     | 35/35 (100%)    | 29 (83%)   | 6 (17%)   | 2           | 13 |
| 12  | M     | 33/33 (100%)    | 28 (85%)   | 5 (15%)   | 3           | 15 |
| 12  | m     | 33/33 (100%)    | 28 (85%)   | 5 (15%)   | 3           | 15 |
| 13  | O     | 206/206 (100%)  | 170 (82%)  | 36 (18%)  | 2           | 13 |
| 13  | o     | 206/206 (100%)  | 170 (82%)  | 36 (18%)  | 2           | 13 |
| 14  | T     | 27/27 (100%)    | 24 (89%)   | 3 (11%)   | 6           | 23 |
| 14  | t     | 27/27 (100%)    | 24 (89%)   | 3 (11%)   | 6           | 23 |
| 15  | U     | 85/85 (100%)    | 74 (87%)   | 11 (13%)  | 4           | 19 |
| 15  | u     | 85/85 (100%)    | 75 (88%)   | 10 (12%)  | 5           | 21 |
| 16  | V     | 117/117 (100%)  | 96 (82%)   | 21 (18%)  | 2           | 12 |
| 16  | v     | 117/117 (100%)  | 97 (83%)   | 20 (17%)  | 2           | 13 |
| 17  | X     | 27/27 (100%)    | 16 (59%)   | 11 (41%)  | 0           | 0  |
| 17  | x     | 27/27 (100%)    | 16 (59%)   | 11 (41%)  | 0           | 0  |
| 18  | Y     | 21/21 (100%)    | 11 (52%)   | 10 (48%)  | 0           | 0  |
| 18  | y     | 21/21 (100%)    | 11 (52%)   | 10 (48%)  | 0           | 0  |
| 20  | Z     | 52/52 (100%)    | 41 (79%)   | 11 (21%)  | 1           | 7  |
| 20  | z     | 52/52 (100%)    | 41 (79%)   | 11 (21%)  | 1           | 7  |
| All | All   | 4250/4296 (99%) | 3434 (81%) | 816 (19%) | 1           | 10 |

All (816) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 1   | A     | 14  | TRP  |
| 1   | A     | 18  | CYS  |
| 1   | A     | 24  | THR  |
| 1   | A     | 28  | LEU  |
| 1   | A     | 30  | VAL  |
| 1   | A     | 35  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 36  | ILE  |
| 1   | A     | 40  | THR  |
| 1   | A     | 42  | LEU  |
| 1   | A     | 63  | ILE  |
| 1   | A     | 70  | SER  |
| 1   | A     | 78  | ILE  |
| 1   | A     | 79  | THR  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 101 | SER  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 119 | PHE  |
| 1   | A     | 126 | TYR  |
| 1   | A     | 127 | MET  |
| 1   | A     | 131 | TRP  |
| 1   | A     | 142 | TRP  |
| 1   | A     | 150 | PRO  |
| 1   | A     | 151 | LEU  |
| 1   | A     | 159 | LEU  |
| 1   | A     | 184 | ILE  |
| 1   | A     | 192 | ILE  |
| 1   | A     | 193 | LEU  |
| 1   | A     | 197 | PHE  |
| 1   | A     | 199 | GLN  |
| 1   | A     | 206 | PHE  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 223 | LEU  |
| 1   | A     | 224 | ILE  |
| 1   | A     | 225 | ARG  |
| 1   | A     | 230 | THR  |
| 1   | A     | 234 | ASN  |
| 1   | A     | 235 | TYR  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 245 | THR  |
| 1   | A     | 246 | TYR  |
| 1   | A     | 254 | TYR  |
| 1   | A     | 267 | ASN  |
| 1   | A     | 268 | SER  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 278 | TRP  |
| 1   | A     | 281 | VAL  |
| 1   | A     | 290 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 297 | LEU  |
| 1   | A     | 298 | ASN  |
| 1   | A     | 303 | ASN  |
| 1   | A     | 313 | VAL  |
| 1   | A     | 317 | TRP  |
| 1   | A     | 325 | ASN  |
| 1   | A     | 331 | MET  |
| 1   | A     | 335 | ASN  |
| 2   | B     | 6   | TYR  |
| 2   | B     | 7   | ARG  |
| 2   | B     | 8   | VAL  |
| 2   | B     | 12  | LEU  |
| 2   | B     | 13  | ILE  |
| 2   | B     | 27  | THR  |
| 2   | B     | 40  | TYR  |
| 2   | B     | 49  | ASP  |
| 2   | B     | 62  | VAL  |
| 2   | B     | 66  | MET  |
| 2   | B     | 68  | ARG  |
| 2   | B     | 69  | LEU  |
| 2   | B     | 71  | VAL  |
| 2   | B     | 75  | TRP  |
| 2   | B     | 81  | THR  |
| 2   | B     | 83  | GLU  |
| 2   | B     | 86  | ILE  |
| 2   | B     | 90  | PHE  |
| 2   | B     | 98  | LEU  |
| 2   | B     | 102 | VAL  |
| 2   | B     | 103 | LEU  |
| 2   | B     | 113 | TRP  |
| 2   | B     | 120 | LEU  |
| 2   | B     | 122 | LEU  |
| 2   | B     | 127 | ARG  |
| 2   | B     | 133 | LEU  |
| 2   | B     | 135 | LEU  |
| 2   | B     | 143 | LEU  |
| 2   | B     | 156 | PHE  |
| 2   | B     | 174 | LEU  |
| 2   | B     | 185 | TRP  |
| 2   | B     | 215 | PHE  |
| 2   | B     | 230 | ARG  |
| 2   | B     | 246 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 247 | PHE  |
| 2   | B     | 262 | THR  |
| 2   | B     | 265 | ILE  |
| 2   | B     | 266 | GLU  |
| 2   | B     | 271 | THR  |
| 2   | B     | 274 | GLN  |
| 2   | B     | 282 | GLN  |
| 2   | B     | 297 | THR  |
| 2   | B     | 321 | LYS  |
| 2   | B     | 334 | ASP  |
| 2   | B     | 338 | GLN  |
| 2   | B     | 350 | GLU  |
| 2   | B     | 355 | PHE  |
| 2   | B     | 357 | ARG  |
| 2   | B     | 359 | MET  |
| 2   | B     | 363 | PHE  |
| 2   | B     | 368 | VAL  |
| 2   | B     | 372 | ASP  |
| 2   | B     | 373 | LYS  |
| 2   | B     | 374 | ASN  |
| 2   | B     | 377 | VAL  |
| 2   | B     | 385 | ARG  |
| 2   | B     | 389 | LYS  |
| 2   | B     | 390 | TYR  |
| 2   | B     | 395 | GLN  |
| 2   | B     | 402 | TYR  |
| 2   | B     | 406 | LEU  |
| 2   | B     | 423 | LYS  |
| 2   | B     | 425 | ILE  |
| 2   | B     | 429 | ILE  |
| 2   | B     | 433 | ASP  |
| 2   | B     | 437 | LEU  |
| 2   | B     | 463 | PHE  |
| 2   | B     | 473 | THR  |
| 2   | B     | 475 | PHE  |
| 2   | B     | 476 | ARG  |
| 2   | B     | 482 | ILE  |
| 2   | B     | 485 | GLU  |
| 2   | B     | 489 | GLU  |
| 3   | C     | 27  | ASP  |
| 3   | C     | 31  | SER  |
| 3   | C     | 33  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 43  | ILE  |
| 3   | C     | 45  | LEU  |
| 3   | C     | 46  | SER  |
| 3   | C     | 48  | LYS  |
| 3   | C     | 49  | LEU  |
| 3   | C     | 50  | LEU  |
| 3   | C     | 56  | HIS  |
| 3   | C     | 67  | MET  |
| 3   | C     | 78  | GLU  |
| 3   | C     | 87  | ILE  |
| 3   | C     | 88  | LEU  |
| 3   | C     | 89  | ILE  |
| 3   | C     | 92  | ILE  |
| 3   | C     | 101 | PRO  |
| 3   | C     | 104 | GLU  |
| 3   | C     | 105 | VAL  |
| 3   | C     | 106 | VAL  |
| 3   | C     | 108 | THR  |
| 3   | C     | 117 | VAL  |
| 3   | C     | 122 | SER  |
| 3   | C     | 125 | LEU  |
| 3   | C     | 134 | ILE  |
| 3   | C     | 141 | GLU  |
| 3   | C     | 146 | PHE  |
| 3   | C     | 149 | TYR  |
| 3   | C     | 152 | LYS  |
| 3   | C     | 156 | LYS  |
| 3   | C     | 160 | ILE  |
| 3   | C     | 161 | LEU  |
| 3   | C     | 166 | ILE  |
| 3   | C     | 167 | VAL  |
| 3   | C     | 170 | ILE  |
| 3   | C     | 174 | LEU  |
| 3   | C     | 175 | LEU  |
| 3   | C     | 191 | PRO  |
| 3   | C     | 223 | TRP  |
| 3   | C     | 228 | ASN  |
| 3   | C     | 229 | ASN  |
| 3   | C     | 240 | ILE  |
| 3   | C     | 244 | CYS  |
| 3   | C     | 257 | PHE  |
| 3   | C     | 264 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 265 | ILE  |
| 3   | C     | 272 | LEU  |
| 3   | C     | 276 | LEU  |
| 3   | C     | 282 | MET  |
| 3   | C     | 288 | CYS  |
| 3   | C     | 295 | THR  |
| 3   | C     | 318 | LEU  |
| 3   | C     | 324 | LEU  |
| 3   | C     | 328 | VAL  |
| 3   | C     | 334 | PRO  |
| 3   | C     | 335 | THR  |
| 3   | C     | 340 | TYR  |
| 3   | C     | 343 | ARG  |
| 3   | C     | 348 | GLU  |
| 3   | C     | 350 | ILE  |
| 3   | C     | 381 | LYS  |
| 3   | C     | 416 | SER  |
| 3   | C     | 417 | VAL  |
| 3   | C     | 418 | ASN  |
| 3   | C     | 419 | PHE  |
| 3   | C     | 420 | VAL  |
| 3   | C     | 436 | PHE  |
| 3   | C     | 441 | HIS  |
| 3   | C     | 443 | TRP  |
| 3   | C     | 456 | GLU  |
| 3   | C     | 467 | LEU  |
| 3   | C     | 472 | LEU  |
| 3   | C     | 473 | ASP  |
| 4   | D     | 14  | TRP  |
| 4   | D     | 17  | ILE  |
| 4   | D     | 24  | ARG  |
| 4   | D     | 25  | ASP  |
| 4   | D     | 30  | VAL  |
| 4   | D     | 32  | TRP  |
| 4   | D     | 36  | LEU  |
| 4   | D     | 37  | LEU  |
| 4   | D     | 43  | LEU  |
| 4   | D     | 50  | THR  |
| 4   | D     | 53  | THR  |
| 4   | D     | 88  | SER  |
| 4   | D     | 89  | LEU  |
| 4   | D     | 102 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 138 | VAL  |
| 4   | D     | 178 | ILE  |
| 4   | D     | 180 | ARG  |
| 4   | D     | 183 | LEU  |
| 4   | D     | 201 | VAL  |
| 4   | D     | 213 | ILE  |
| 4   | D     | 218 | VAL  |
| 4   | D     | 222 | LEU  |
| 4   | D     | 225 | ASP  |
| 4   | D     | 232 | PHE  |
| 4   | D     | 247 | VAL  |
| 4   | D     | 250 | ASN  |
| 4   | D     | 265 | ARG  |
| 4   | D     | 272 | LEU  |
| 4   | D     | 277 | THR  |
| 4   | D     | 282 | SER  |
| 4   | D     | 287 | VAL  |
| 4   | D     | 295 | SER  |
| 4   | D     | 298 | PHE  |
| 4   | D     | 311 | PHE  |
| 4   | D     | 316 | THR  |
| 4   | D     | 320 | LEU  |
| 4   | D     | 337 | GLU  |
| 4   | D     | 338 | ASN  |
| 4   | D     | 345 | VAL  |
| 4   | D     | 352 | LEU  |
| 5   | E     | 15  | THR  |
| 5   | E     | 17  | VAL  |
| 5   | E     | 24  | SER  |
| 5   | E     | 27  | ILE  |
| 5   | E     | 32  | ILE  |
| 5   | E     | 39  | SER  |
| 5   | E     | 42  | LEU  |
| 5   | E     | 45  | ASP  |
| 5   | E     | 52  | PRO  |
| 5   | E     | 58  | GLN  |
| 5   | E     | 60  | GLN  |
| 5   | E     | 63  | ILE  |
| 5   | E     | 65  | LEU  |
| 5   | E     | 75  | GLN  |
| 5   | E     | 76  | VAL  |
| 6   | F     | 11  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 17  | THR  |
| 6   | F     | 19  | ARG  |
| 6   | F     | 24  | HIS  |
| 6   | F     | 32  | PHE  |
| 6   | F     | 43  | ILE  |
| 6   | F     | 45  | ARG  |
| 7   | H     | 4   | ARG  |
| 7   | H     | 17  | GLU  |
| 7   | H     | 27  | THR  |
| 7   | H     | 35  | MET  |
| 7   | H     | 39  | LEU  |
| 7   | H     | 43  | LEU  |
| 7   | H     | 44  | ILE  |
| 7   | H     | 52  | THR  |
| 7   | H     | 53  | LEU  |
| 8   | I     | 6   | ILE  |
| 8   | I     | 8   | VAL  |
| 8   | I     | 10  | ILE  |
| 8   | I     | 12  | VAL  |
| 8   | I     | 14  | PHE  |
| 8   | I     | 20  | VAL  |
| 8   | I     | 23  | PHE  |
| 8   | I     | 33  | LYS  |
| 9   | J     | 10  | LEU  |
| 9   | J     | 11  | TRP  |
| 9   | J     | 12  | ILE  |
| 9   | J     | 21  | VAL  |
| 9   | J     | 25  | VAL  |
| 9   | J     | 38  | SER  |
| 10  | K     | 12  | PRO  |
| 10  | K     | 17  | ILE  |
| 10  | K     | 21  | LEU  |
| 10  | K     | 23  | ASP  |
| 10  | K     | 33  | PHE  |
| 10  | K     | 38  | VAL  |
| 10  | K     | 39  | VAL  |
| 10  | K     | 40  | GLN  |
| 11  | L     | 8   | GLN  |
| 11  | L     | 11  | GLU  |
| 11  | L     | 15  | THR  |
| 11  | L     | 17  | LEU  |
| 11  | L     | 26  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | L     | 30  | LEU  |
| 12  | M     | 3   | VAL  |
| 12  | M     | 11  | THR  |
| 12  | M     | 17  | VAL  |
| 12  | M     | 25  | LEU  |
| 12  | M     | 28  | GLN  |
| 13  | O     | 41  | LEU  |
| 13  | O     | 46  | PRO  |
| 13  | O     | 47  | THR  |
| 13  | O     | 49  | ASP  |
| 13  | O     | 58  | ILE  |
| 13  | O     | 69  | LEU  |
| 13  | O     | 73  | PRO  |
| 13  | O     | 83  | LYS  |
| 13  | O     | 84  | ASN  |
| 13  | O     | 85  | LYS  |
| 13  | O     | 86  | ARG  |
| 13  | O     | 87  | GLN  |
| 13  | O     | 90  | GLU  |
| 13  | O     | 91  | PHE  |
| 13  | O     | 99  | ARG  |
| 13  | O     | 101 | THR  |
| 13  | O     | 102 | THR  |
| 13  | O     | 113 | VAL  |
| 13  | O     | 116 | ASP  |
| 13  | O     | 125 | ASP  |
| 13  | O     | 130 | GLN  |
| 13  | O     | 136 | MET  |
| 13  | O     | 140 | GLU  |
| 13  | O     | 141 | ARG  |
| 13  | O     | 160 | THR  |
| 13  | O     | 173 | ASN  |
| 13  | O     | 176 | SER  |
| 13  | O     | 181 | ASN  |
| 13  | O     | 183 | LEU  |
| 13  | O     | 186 | LYS  |
| 13  | O     | 194 | TYR  |
| 13  | O     | 195 | ASP  |
| 13  | O     | 213 | VAL  |
| 13  | O     | 223 | ILE  |
| 13  | O     | 237 | ILE  |
| 13  | O     | 264 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | T     | 2   | GLU  |
| 14  | T     | 4   | ILE  |
| 14  | T     | 12  | CYS  |
| 15  | U     | 9   | LEU  |
| 15  | U     | 31  | ASN  |
| 15  | U     | 60  | ASP  |
| 15  | U     | 63  | ASN  |
| 15  | U     | 64  | ILE  |
| 15  | U     | 68  | THR  |
| 15  | U     | 69  | GLU  |
| 15  | U     | 79  | LEU  |
| 15  | U     | 82  | PHE  |
| 15  | U     | 87  | VAL  |
| 15  | U     | 89  | THR  |
| 16  | V     | 34  | LEU  |
| 16  | V     | 38  | LEU  |
| 16  | V     | 44  | THR  |
| 16  | V     | 45  | ILE  |
| 16  | V     | 47  | LEU  |
| 16  | V     | 49  | GLU  |
| 16  | V     | 63  | CYS  |
| 16  | V     | 65  | SER  |
| 16  | V     | 66  | CYS  |
| 16  | V     | 67  | HIS  |
| 16  | V     | 68  | VAL  |
| 16  | V     | 81  | ARG  |
| 16  | V     | 83  | GLU  |
| 16  | V     | 92  | ARG  |
| 16  | V     | 103 | LYS  |
| 16  | V     | 106 | THR  |
| 16  | V     | 114 | ILE  |
| 16  | V     | 119 | PRO  |
| 16  | V     | 126 | ILE  |
| 16  | V     | 151 | ILE  |
| 16  | V     | 156 | TRP  |
| 17  | X     | 12  | ILE  |
| 17  | X     | 13  | THR  |
| 17  | X     | 15  | SER  |
| 17  | X     | 24  | LEU  |
| 17  | X     | 29  | VAL  |
| 17  | X     | 32  | LEU  |
| 17  | X     | 33  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | X     | 36   | VAL  |
| 17  | X     | 37   | LEU  |
| 17  | X     | 41   | SER  |
| 17  | X     | 42   | GLN  |
| 18  | Y     | 22   | LEU  |
| 18  | Y     | 25   | ILE  |
| 18  | Y     | 28   | ILE  |
| 18  | Y     | 30   | ILE  |
| 18  | Y     | 35   | ILE  |
| 18  | Y     | 36   | ILE  |
| 18  | Y     | 41   | VAL  |
| 18  | Y     | 42   | ARG  |
| 18  | Y     | 43   | ARG  |
| 18  | Y     | 45   | ASN  |
| 20  | Z     | 1    | MET  |
| 20  | Z     | 2    | THR  |
| 20  | Z     | 4    | LEU  |
| 20  | Z     | 6    | GLN  |
| 20  | Z     | 15   | LEU  |
| 20  | Z     | 24   | PRO  |
| 20  | Z     | 27   | TYR  |
| 20  | Z     | 32   | ASP  |
| 20  | Z     | 38   | GLN  |
| 20  | Z     | 50   | LEU  |
| 20  | Z     | 60   | PHE  |
| 1   | a     | 5012 | ASN  |
| 1   | a     | 5014 | TRP  |
| 1   | a     | 5018 | CYS  |
| 1   | a     | 5024 | THR  |
| 1   | a     | 5028 | LEU  |
| 1   | a     | 5030 | VAL  |
| 1   | a     | 5035 | VAL  |
| 1   | a     | 5036 | ILE  |
| 1   | a     | 5040 | THR  |
| 1   | a     | 5042 | LEU  |
| 1   | a     | 5063 | ILE  |
| 1   | a     | 5070 | SER  |
| 1   | a     | 5078 | ILE  |
| 1   | a     | 5079 | THR  |
| 1   | a     | 5083 | VAL  |
| 1   | a     | 5101 | SER  |
| 1   | a     | 5102 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 5114 | LEU  |
| 1   | a     | 5119 | PHE  |
| 1   | a     | 5126 | TYR  |
| 1   | a     | 5127 | MET  |
| 1   | a     | 5131 | TRP  |
| 1   | a     | 5142 | TRP  |
| 1   | a     | 5150 | PRO  |
| 1   | a     | 5151 | LEU  |
| 1   | a     | 5159 | LEU  |
| 1   | a     | 5184 | ILE  |
| 1   | a     | 5192 | ILE  |
| 1   | a     | 5193 | LEU  |
| 1   | a     | 5197 | PHE  |
| 1   | a     | 5199 | GLN  |
| 1   | a     | 5206 | PHE  |
| 1   | a     | 5218 | LEU  |
| 1   | a     | 5223 | LEU  |
| 1   | a     | 5224 | ILE  |
| 1   | a     | 5225 | ARG  |
| 1   | a     | 5230 | THR  |
| 1   | a     | 5234 | ASN  |
| 1   | a     | 5235 | TYR  |
| 1   | a     | 5243 | GLU  |
| 1   | a     | 5245 | THR  |
| 1   | a     | 5246 | TYR  |
| 1   | a     | 5267 | ASN  |
| 1   | a     | 5268 | SER  |
| 1   | a     | 5271 | LEU  |
| 1   | a     | 5278 | TRP  |
| 1   | a     | 5279 | ARG  |
| 1   | a     | 5281 | VAL  |
| 1   | a     | 5290 | ILE  |
| 1   | a     | 5297 | LEU  |
| 1   | a     | 5298 | ASN  |
| 1   | a     | 5303 | ASN  |
| 1   | a     | 5313 | VAL  |
| 1   | a     | 5317 | TRP  |
| 1   | a     | 5325 | ASN  |
| 1   | a     | 5331 | MET  |
| 1   | a     | 5335 | ASN  |
| 2   | b     | 5006 | TYR  |
| 2   | b     | 5007 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | b     | 5008 | VAL  |
| 2   | b     | 5012 | LEU  |
| 2   | b     | 5013 | ILE  |
| 2   | b     | 5027 | THR  |
| 2   | b     | 5040 | TYR  |
| 2   | b     | 5049 | ASP  |
| 2   | b     | 5062 | VAL  |
| 2   | b     | 5066 | MET  |
| 2   | b     | 5068 | ARG  |
| 2   | b     | 5069 | LEU  |
| 2   | b     | 5071 | VAL  |
| 2   | b     | 5075 | TRP  |
| 2   | b     | 5081 | THR  |
| 2   | b     | 5083 | GLU  |
| 2   | b     | 5086 | ILE  |
| 2   | b     | 5090 | PHE  |
| 2   | b     | 5098 | LEU  |
| 2   | b     | 5102 | VAL  |
| 2   | b     | 5103 | LEU  |
| 2   | b     | 5113 | TRP  |
| 2   | b     | 5120 | LEU  |
| 2   | b     | 5122 | LEU  |
| 2   | b     | 5127 | ARG  |
| 2   | b     | 5133 | LEU  |
| 2   | b     | 5135 | LEU  |
| 2   | b     | 5143 | LEU  |
| 2   | b     | 5156 | PHE  |
| 2   | b     | 5174 | LEU  |
| 2   | b     | 5185 | TRP  |
| 2   | b     | 5215 | PHE  |
| 2   | b     | 5230 | ARG  |
| 2   | b     | 5246 | PHE  |
| 2   | b     | 5247 | PHE  |
| 2   | b     | 5262 | THR  |
| 2   | b     | 5265 | ILE  |
| 2   | b     | 5266 | GLU  |
| 2   | b     | 5271 | THR  |
| 2   | b     | 5274 | GLN  |
| 2   | b     | 5282 | GLN  |
| 2   | b     | 5297 | THR  |
| 2   | b     | 5321 | LYS  |
| 2   | b     | 5334 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | b     | 5338 | GLN  |
| 2   | b     | 5350 | GLU  |
| 2   | b     | 5355 | PHE  |
| 2   | b     | 5357 | ARG  |
| 2   | b     | 5359 | MET  |
| 2   | b     | 5363 | PHE  |
| 2   | b     | 5368 | VAL  |
| 2   | b     | 5372 | ASP  |
| 2   | b     | 5373 | LYS  |
| 2   | b     | 5374 | ASN  |
| 2   | b     | 5377 | VAL  |
| 2   | b     | 5385 | ARG  |
| 2   | b     | 5389 | LYS  |
| 2   | b     | 5390 | TYR  |
| 2   | b     | 5395 | GLN  |
| 2   | b     | 5402 | TYR  |
| 2   | b     | 5406 | LEU  |
| 2   | b     | 5423 | LYS  |
| 2   | b     | 5425 | ILE  |
| 2   | b     | 5429 | ILE  |
| 2   | b     | 5433 | ASP  |
| 2   | b     | 5437 | LEU  |
| 2   | b     | 5463 | PHE  |
| 2   | b     | 5473 | THR  |
| 2   | b     | 5475 | PHE  |
| 2   | b     | 5476 | ARG  |
| 2   | b     | 5482 | ILE  |
| 2   | b     | 5485 | GLU  |
| 2   | b     | 5489 | GLU  |
| 3   | c     | 5027 | ASP  |
| 3   | c     | 5031 | SER  |
| 3   | c     | 5033 | PHE  |
| 3   | c     | 5042 | LEU  |
| 3   | c     | 5043 | ILE  |
| 3   | c     | 5045 | LEU  |
| 3   | c     | 5046 | SER  |
| 3   | c     | 5048 | LYS  |
| 3   | c     | 5049 | LEU  |
| 3   | c     | 5050 | LEU  |
| 3   | c     | 5056 | HIS  |
| 3   | c     | 5067 | MET  |
| 3   | c     | 5078 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | c     | 5088 | LEU  |
| 3   | c     | 5089 | ILE  |
| 3   | c     | 5092 | ILE  |
| 3   | c     | 5101 | PRO  |
| 3   | c     | 5104 | GLU  |
| 3   | c     | 5105 | VAL  |
| 3   | c     | 5106 | VAL  |
| 3   | c     | 5108 | THR  |
| 3   | c     | 5117 | VAL  |
| 3   | c     | 5122 | SER  |
| 3   | c     | 5125 | LEU  |
| 3   | c     | 5134 | ILE  |
| 3   | c     | 5141 | GLU  |
| 3   | c     | 5146 | PHE  |
| 3   | c     | 5149 | TYR  |
| 3   | c     | 5152 | LYS  |
| 3   | c     | 5156 | LYS  |
| 3   | c     | 5160 | ILE  |
| 3   | c     | 5161 | LEU  |
| 3   | c     | 5166 | ILE  |
| 3   | c     | 5167 | VAL  |
| 3   | c     | 5170 | ILE  |
| 3   | c     | 5174 | LEU  |
| 3   | c     | 5175 | LEU  |
| 3   | c     | 5191 | PRO  |
| 3   | c     | 5223 | TRP  |
| 3   | c     | 5228 | ASN  |
| 3   | c     | 5229 | ASN  |
| 3   | c     | 5240 | ILE  |
| 3   | c     | 5244 | CYS  |
| 3   | c     | 5257 | PHE  |
| 3   | c     | 5264 | PHE  |
| 3   | c     | 5265 | ILE  |
| 3   | c     | 5272 | LEU  |
| 3   | c     | 5276 | LEU  |
| 3   | c     | 5282 | MET  |
| 3   | c     | 5288 | CYS  |
| 3   | c     | 5295 | THR  |
| 3   | c     | 5318 | LEU  |
| 3   | c     | 5324 | LEU  |
| 3   | c     | 5328 | VAL  |
| 3   | c     | 5334 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | c     | 5335 | THR  |
| 3   | c     | 5340 | TYR  |
| 3   | c     | 5343 | ARG  |
| 3   | c     | 5348 | GLU  |
| 3   | c     | 5350 | ILE  |
| 3   | c     | 5381 | LYS  |
| 3   | c     | 5416 | SER  |
| 3   | c     | 5417 | VAL  |
| 3   | c     | 5418 | ASN  |
| 3   | c     | 5419 | PHE  |
| 3   | c     | 5420 | VAL  |
| 3   | c     | 5436 | PHE  |
| 3   | c     | 5441 | HIS  |
| 3   | c     | 5443 | TRP  |
| 3   | c     | 5456 | GLU  |
| 3   | c     | 5467 | LEU  |
| 3   | c     | 5472 | LEU  |
| 3   | c     | 5473 | ASP  |
| 4   | d     | 5014 | TRP  |
| 4   | d     | 5017 | ILE  |
| 4   | d     | 5024 | ARG  |
| 4   | d     | 5025 | ASP  |
| 4   | d     | 5030 | VAL  |
| 4   | d     | 5032 | TRP  |
| 4   | d     | 5036 | LEU  |
| 4   | d     | 5037 | LEU  |
| 4   | d     | 5043 | LEU  |
| 4   | d     | 5050 | THR  |
| 4   | d     | 5053 | THR  |
| 4   | d     | 5088 | SER  |
| 4   | d     | 5089 | LEU  |
| 4   | d     | 5102 | THR  |
| 4   | d     | 5138 | VAL  |
| 4   | d     | 5178 | ILE  |
| 4   | d     | 5180 | ARG  |
| 4   | d     | 5183 | LEU  |
| 4   | d     | 5201 | VAL  |
| 4   | d     | 5213 | ILE  |
| 4   | d     | 5218 | VAL  |
| 4   | d     | 5222 | LEU  |
| 4   | d     | 5225 | ASP  |
| 4   | d     | 5232 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | d     | 5247 | VAL  |
| 4   | d     | 5250 | ASN  |
| 4   | d     | 5265 | ARG  |
| 4   | d     | 5272 | LEU  |
| 4   | d     | 5277 | THR  |
| 4   | d     | 5282 | SER  |
| 4   | d     | 5287 | VAL  |
| 4   | d     | 5295 | SER  |
| 4   | d     | 5298 | PHE  |
| 4   | d     | 5311 | PHE  |
| 4   | d     | 5316 | THR  |
| 4   | d     | 5320 | LEU  |
| 4   | d     | 5337 | GLU  |
| 4   | d     | 5338 | ASN  |
| 4   | d     | 5345 | VAL  |
| 4   | d     | 5352 | LEU  |
| 5   | e     | 5015 | THR  |
| 5   | e     | 5017 | VAL  |
| 5   | e     | 5024 | SER  |
| 5   | e     | 5027 | ILE  |
| 5   | e     | 5032 | ILE  |
| 5   | e     | 5039 | SER  |
| 5   | e     | 5042 | LEU  |
| 5   | e     | 5045 | ASP  |
| 5   | e     | 5052 | PRO  |
| 5   | e     | 5058 | GLN  |
| 5   | e     | 5060 | GLN  |
| 5   | e     | 5063 | ILE  |
| 5   | e     | 5065 | LEU  |
| 5   | e     | 5075 | GLN  |
| 5   | e     | 5076 | VAL  |
| 6   | f     | 5011 | VAL  |
| 6   | f     | 5017 | THR  |
| 6   | f     | 5019 | ARG  |
| 6   | f     | 5024 | HIS  |
| 6   | f     | 5032 | PHE  |
| 6   | f     | 5043 | ILE  |
| 6   | f     | 5045 | ARG  |
| 7   | h     | 5004 | ARG  |
| 7   | h     | 5017 | GLU  |
| 7   | h     | 5027 | THR  |
| 7   | h     | 5035 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | h     | 5039 | LEU  |
| 7   | h     | 5043 | LEU  |
| 7   | h     | 5044 | ILE  |
| 7   | h     | 5052 | THR  |
| 7   | h     | 5053 | LEU  |
| 8   | i     | 5006 | ILE  |
| 8   | i     | 5008 | VAL  |
| 8   | i     | 5010 | ILE  |
| 8   | i     | 5012 | VAL  |
| 8   | i     | 5014 | PHE  |
| 8   | i     | 5020 | VAL  |
| 8   | i     | 5023 | PHE  |
| 8   | i     | 5033 | LYS  |
| 9   | j     | 5010 | LEU  |
| 9   | j     | 5011 | TRP  |
| 9   | j     | 5012 | ILE  |
| 9   | j     | 5021 | VAL  |
| 9   | j     | 5025 | VAL  |
| 9   | j     | 5038 | SER  |
| 10  | k     | 5012 | PRO  |
| 10  | k     | 5017 | ILE  |
| 10  | k     | 5021 | LEU  |
| 10  | k     | 5023 | ASP  |
| 10  | k     | 5033 | PHE  |
| 10  | k     | 5038 | VAL  |
| 11  | l     | 5008 | GLN  |
| 11  | l     | 5011 | GLU  |
| 11  | l     | 5015 | THR  |
| 11  | l     | 5017 | LEU  |
| 11  | l     | 5026 | VAL  |
| 11  | l     | 5030 | LEU  |
| 12  | m     | 5003 | VAL  |
| 12  | m     | 5011 | THR  |
| 12  | m     | 5017 | VAL  |
| 12  | m     | 5025 | LEU  |
| 12  | m     | 5028 | GLN  |
| 13  | o     | 5041 | LEU  |
| 13  | o     | 5046 | PRO  |
| 13  | o     | 5047 | THR  |
| 13  | o     | 5049 | ASP  |
| 13  | o     | 5058 | ILE  |
| 13  | o     | 5069 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 13  | o     | 5073 | PRO  |
| 13  | o     | 5083 | LYS  |
| 13  | o     | 5084 | ASN  |
| 13  | o     | 5085 | LYS  |
| 13  | o     | 5086 | ARG  |
| 13  | o     | 5087 | GLN  |
| 13  | o     | 5090 | GLU  |
| 13  | o     | 5091 | PHE  |
| 13  | o     | 5099 | ARG  |
| 13  | o     | 5101 | THR  |
| 13  | o     | 5102 | THR  |
| 13  | o     | 5113 | VAL  |
| 13  | o     | 5116 | ASP  |
| 13  | o     | 5125 | ASP  |
| 13  | o     | 5130 | GLN  |
| 13  | o     | 5136 | MET  |
| 13  | o     | 5140 | GLU  |
| 13  | o     | 5141 | ARG  |
| 13  | o     | 5160 | THR  |
| 13  | o     | 5173 | ASN  |
| 13  | o     | 5176 | SER  |
| 13  | o     | 5181 | ASN  |
| 13  | o     | 5183 | LEU  |
| 13  | o     | 5186 | LYS  |
| 13  | o     | 5194 | TYR  |
| 13  | o     | 5195 | ASP  |
| 13  | o     | 5213 | VAL  |
| 13  | o     | 5223 | ILE  |
| 13  | o     | 5237 | ILE  |
| 13  | o     | 5264 | VAL  |
| 14  | t     | 5002 | GLU  |
| 14  | t     | 5004 | ILE  |
| 14  | t     | 5012 | CYS  |
| 15  | u     | 5009 | LEU  |
| 15  | u     | 5031 | ASN  |
| 15  | u     | 5060 | ASP  |
| 15  | u     | 5064 | ILE  |
| 15  | u     | 5068 | THR  |
| 15  | u     | 5069 | GLU  |
| 15  | u     | 5079 | LEU  |
| 15  | u     | 5082 | PHE  |
| 15  | u     | 5087 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | u     | 5089 | THR  |
| 16  | v     | 5034 | LEU  |
| 16  | v     | 5038 | LEU  |
| 16  | v     | 5044 | THR  |
| 16  | v     | 5045 | ILE  |
| 16  | v     | 5047 | LEU  |
| 16  | v     | 5049 | GLU  |
| 16  | v     | 5063 | CYS  |
| 16  | v     | 5065 | SER  |
| 16  | v     | 5066 | CYS  |
| 16  | v     | 5067 | HIS  |
| 16  | v     | 5068 | VAL  |
| 16  | v     | 5081 | ARG  |
| 16  | v     | 5083 | GLU  |
| 16  | v     | 5092 | ARG  |
| 16  | v     | 5106 | THR  |
| 16  | v     | 5114 | ILE  |
| 16  | v     | 5119 | PRO  |
| 16  | v     | 5126 | ILE  |
| 16  | v     | 5151 | ILE  |
| 16  | v     | 5156 | TRP  |
| 17  | x     | 5012 | ILE  |
| 17  | x     | 5013 | THR  |
| 17  | x     | 5015 | SER  |
| 17  | x     | 5024 | LEU  |
| 17  | x     | 5029 | VAL  |
| 17  | x     | 5032 | LEU  |
| 17  | x     | 5033 | THR  |
| 17  | x     | 5036 | VAL  |
| 17  | x     | 5037 | LEU  |
| 17  | x     | 5041 | SER  |
| 17  | x     | 5042 | GLN  |
| 18  | y     | 5022 | LEU  |
| 18  | y     | 5025 | ILE  |
| 18  | y     | 5028 | ILE  |
| 18  | y     | 5030 | ILE  |
| 18  | y     | 5035 | ILE  |
| 18  | y     | 5036 | ILE  |
| 18  | y     | 5041 | VAL  |
| 18  | y     | 5042 | ARG  |
| 18  | y     | 5043 | ARG  |
| 18  | y     | 5045 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | z     | 5001 | MET  |
| 20  | z     | 5002 | THR  |
| 20  | z     | 5004 | LEU  |
| 20  | z     | 5006 | GLN  |
| 20  | z     | 5015 | LEU  |
| 20  | z     | 5024 | PRO  |
| 20  | z     | 5027 | TYR  |
| 20  | z     | 5032 | ASP  |
| 20  | z     | 5038 | GLN  |
| 20  | z     | 5050 | LEU  |
| 20  | z     | 5060 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 1   | A     | 19  | ASN  |
| 1   | A     | 26  | ASN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 92  | HIS  |
| 1   | A     | 118 | HIS  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 198 | HIS  |
| 1   | A     | 199 | GLN  |
| 1   | A     | 241 | GLN  |
| 1   | A     | 247 | ASN  |
| 1   | A     | 267 | ASN  |
| 1   | A     | 272 | HIS  |
| 1   | A     | 296 | ASN  |
| 1   | A     | 298 | ASN  |
| 1   | A     | 303 | ASN  |
| 1   | A     | 312 | ASN  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 325 | ASN  |
| 1   | A     | 337 | HIS  |
| 2   | B     | 23  | HIS  |
| 2   | B     | 53  | ASN  |
| 2   | B     | 58  | GLN  |
| 2   | B     | 114 | HIS  |
| 2   | B     | 157 | HIS  |
| 2   | B     | 191 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 201 | HIS  |
| 2   | B     | 223 | GLN  |
| 2   | B     | 233 | ASN  |
| 2   | B     | 274 | GLN  |
| 2   | B     | 281 | GLN  |
| 2   | B     | 282 | GLN  |
| 2   | B     | 318 | ASN  |
| 2   | B     | 331 | ASN  |
| 2   | B     | 338 | GLN  |
| 2   | B     | 374 | ASN  |
| 2   | B     | 395 | GLN  |
| 2   | B     | 409 | GLN  |
| 3   | C     | 56  | HIS  |
| 3   | C     | 91  | HIS  |
| 3   | C     | 155 | ASN  |
| 3   | C     | 201 | ASN  |
| 3   | C     | 229 | ASN  |
| 3   | C     | 294 | ASN  |
| 3   | C     | 322 | GLN  |
| 3   | C     | 327 | ASN  |
| 3   | C     | 332 | GLN  |
| 3   | C     | 378 | ASN  |
| 3   | C     | 382 | ASN  |
| 3   | C     | 415 | ASN  |
| 4   | D     | 83  | ASN  |
| 4   | D     | 98  | GLN  |
| 4   | D     | 106 | GLN  |
| 4   | D     | 186 | GLN  |
| 4   | D     | 190 | ASN  |
| 4   | D     | 197 | HIS  |
| 4   | D     | 214 | HIS  |
| 4   | D     | 220 | ASN  |
| 4   | D     | 224 | GLN  |
| 4   | D     | 239 | GLN  |
| 4   | D     | 255 | GLN  |
| 4   | D     | 292 | ASN  |
| 4   | D     | 301 | GLN  |
| 4   | D     | 322 | ASN  |
| 4   | D     | 332 | GLN  |
| 4   | D     | 334 | GLN  |
| 5   | E     | 75  | GLN  |
| 6   | F     | 24  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | H     | 15   | ASN  |
| 8   | I     | 31   | ASN  |
| 10  | K     | 40   | GLN  |
| 11  | L     | 4    | ASN  |
| 11  | L     | 6    | ASN  |
| 11  | L     | 8    | GLN  |
| 11  | L     | 37   | ASN  |
| 12  | M     | 28   | GLN  |
| 12  | M     | 32   | GLN  |
| 13  | O     | 62   | GLN  |
| 13  | O     | 72   | GLN  |
| 13  | O     | 84   | ASN  |
| 13  | O     | 114  | ASN  |
| 13  | O     | 150  | ASN  |
| 13  | O     | 173  | ASN  |
| 13  | O     | 254  | HIS  |
| 13  | O     | 262  | GLN  |
| 15  | U     | 28   | ASN  |
| 15  | U     | 29   | ASN  |
| 15  | U     | 31   | ASN  |
| 15  | U     | 78   | ASN  |
| 15  | U     | 81   | HIS  |
| 15  | U     | 99   | ASN  |
| 16  | V     | 39   | ASN  |
| 16  | V     | 51   | GLN  |
| 16  | V     | 60   | GLN  |
| 16  | V     | 67   | HIS  |
| 16  | V     | 94   | ASN  |
| 16  | V     | 104  | ASN  |
| 16  | V     | 112  | GLN  |
| 18  | Y     | 45   | ASN  |
| 20  | Z     | 6    | GLN  |
| 20  | Z     | 31   | GLN  |
| 20  | Z     | 38   | GLN  |
| 1   | a     | 5012 | ASN  |
| 1   | a     | 5019 | ASN  |
| 1   | a     | 5026 | ASN  |
| 1   | a     | 5075 | ASN  |
| 1   | a     | 5087 | ASN  |
| 1   | a     | 5092 | HIS  |
| 1   | a     | 5118 | HIS  |
| 1   | a     | 5181 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 5198 | HIS  |
| 1   | a     | 5199 | GLN  |
| 1   | a     | 5241 | GLN  |
| 1   | a     | 5247 | ASN  |
| 1   | a     | 5267 | ASN  |
| 1   | a     | 5296 | ASN  |
| 1   | a     | 5298 | ASN  |
| 1   | a     | 5303 | ASN  |
| 1   | a     | 5312 | ASN  |
| 1   | a     | 5322 | ASN  |
| 1   | a     | 5325 | ASN  |
| 2   | b     | 5023 | HIS  |
| 2   | b     | 5053 | ASN  |
| 2   | b     | 5114 | HIS  |
| 2   | b     | 5157 | HIS  |
| 2   | b     | 5191 | ASN  |
| 2   | b     | 5201 | HIS  |
| 2   | b     | 5223 | GLN  |
| 2   | b     | 5233 | ASN  |
| 2   | b     | 5274 | GLN  |
| 2   | b     | 5281 | GLN  |
| 2   | b     | 5282 | GLN  |
| 2   | b     | 5318 | ASN  |
| 2   | b     | 5331 | ASN  |
| 2   | b     | 5338 | GLN  |
| 2   | b     | 5374 | ASN  |
| 2   | b     | 5395 | GLN  |
| 3   | c     | 5056 | HIS  |
| 3   | c     | 5091 | HIS  |
| 3   | c     | 5155 | ASN  |
| 3   | c     | 5201 | ASN  |
| 3   | c     | 5229 | ASN  |
| 3   | c     | 5294 | ASN  |
| 3   | c     | 5322 | GLN  |
| 3   | c     | 5327 | ASN  |
| 3   | c     | 5332 | GLN  |
| 3   | c     | 5378 | ASN  |
| 3   | c     | 5382 | ASN  |
| 3   | c     | 5415 | ASN  |
| 4   | d     | 5083 | ASN  |
| 4   | d     | 5098 | GLN  |
| 4   | d     | 5106 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | d     | 5186 | GLN  |
| 4   | d     | 5190 | ASN  |
| 4   | d     | 5197 | HIS  |
| 4   | d     | 5220 | ASN  |
| 4   | d     | 5224 | GLN  |
| 4   | d     | 5239 | GLN  |
| 4   | d     | 5255 | GLN  |
| 4   | d     | 5292 | ASN  |
| 4   | d     | 5301 | GLN  |
| 4   | d     | 5322 | ASN  |
| 4   | d     | 5332 | GLN  |
| 4   | d     | 5334 | GLN  |
| 4   | d     | 5350 | ASN  |
| 5   | e     | 5075 | GLN  |
| 6   | f     | 5024 | HIS  |
| 7   | h     | 5015 | ASN  |
| 8   | i     | 5031 | ASN  |
| 10  | k     | 5040 | GLN  |
| 11  | l     | 5004 | ASN  |
| 11  | l     | 5006 | ASN  |
| 11  | l     | 5008 | GLN  |
| 11  | l     | 5037 | ASN  |
| 12  | m     | 5028 | GLN  |
| 12  | m     | 5032 | GLN  |
| 13  | o     | 5062 | GLN  |
| 13  | o     | 5072 | GLN  |
| 13  | o     | 5084 | ASN  |
| 13  | o     | 5150 | ASN  |
| 13  | o     | 5158 | ASN  |
| 13  | o     | 5173 | ASN  |
| 13  | o     | 5254 | HIS  |
| 13  | o     | 5262 | GLN  |
| 15  | u     | 5028 | ASN  |
| 15  | u     | 5029 | ASN  |
| 15  | u     | 5031 | ASN  |
| 15  | u     | 5078 | ASN  |
| 15  | u     | 5081 | HIS  |
| 15  | u     | 5099 | ASN  |
| 16  | v     | 5039 | ASN  |
| 16  | v     | 5051 | GLN  |
| 16  | v     | 5060 | GLN  |
| 16  | v     | 5067 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | v     | 5094 | ASN  |
| 16  | v     | 5104 | ASN  |
| 16  | v     | 5112 | GLN  |
| 18  | y     | 5045 | ASN  |
| 20  | z     | 5006 | GLN  |
| 20  | z     | 5031 | GLN  |
| 20  | z     | 5038 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 136 ligands modelled in this entry, 12 are monoatomic - leaving 124 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 22  | CLA  | a     | 6003 | -    | 69,73,73     | 1.94 | 16 (23%)    | 82,113,113  | 2.48 | 28 (34%)    |
| 23  | PHO  | a     | 6038 | -    | 58,69,69     | 2.94 | 13 (22%)    | 55,99,99    | 3.53 | 19 (34%)    |
| 22  | CLA  | B     | 1013 | -    | 69,73,73     | 1.94 | 16 (23%)    | 82,113,113  | 2.48 | 28 (34%)    |
| 24  | PQ9  | D     | 1042 | -    | 45,45,45     | 0.68 | 2 (4%)      | 56,57,57    | 1.79 | 17 (30%)    |
| 22  | CLA  | c     | 6026 | -    | 69,73,73     | 1.93 | 15 (21%)    | 82,113,113  | 2.48 | 28 (34%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | A     | 1006 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 29  | DGD  | c     | 6056 | -    | 67,67,67     | 0.85 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 22  | CLA  | b     | 6014 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 31  | HEM  | v     | 6041 | 16   | 50,50,50     | 1.88 | 8 (16%)  | 67,82,82    | 1.36 | 5 (7%)   |
| 25  | BCR  | t     | 1046 | -    | 41,41,41     | 3.96 | 17 (41%) | 56,56,56    | 6.06 | 26 (46%) |
| 22  | CLA  | a     | 6006 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 23  | PHO  | A     | 1038 | -    | 58,69,69     | 2.94 | 13 (22%) | 55,99,99    | 3.53 | 19 (34%) |
| 22  | CLA  | D     | 1005 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 28  | MGE  | D     | 1062 | -    | 48,48,48     | 0.97 | 2 (4%)   | 56,56,56    | 1.02 | 3 (5%)   |
| 25  | BCR  | b     | 6045 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 6.17 | 20 (35%) |
| 25  | BCR  | k     | 6052 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 6.97 | 24 (42%) |
| 22  | CLA  | B     | 1020 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | D     | 1008 | -    | 69,73,73     | 1.92 | 17 (24%) | 82,113,113  | 2.48 | 29 (35%) |
| 22  | CLA  | B     | 1015 | -    | 69,73,73     | 1.93 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | C     | 1031 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | B     | 1016 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | C     | 1032 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | k     | 6034 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.49 | 28 (34%) |
| 25  | BCR  | C     | 1052 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 6.97 | 24 (42%) |
| 22  | CLA  | B     | 1018 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | B     | 1021 | 2    | 69,73,73     | 1.92 | 16 (23%) | 82,113,113  | 2.49 | 30 (36%) |
| 26  | LHG  | A     | 1063 | -    | 48,48,48     | 0.95 | 2 (4%)   | 51,54,54    | 1.05 | 3 (5%)   |
| 22  | CLA  | b     | 6024 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.47 | 28 (34%) |
| 22  | CLA  | b     | 6011 | -    | 69,73,73     | 1.92 | 17 (24%) | 82,113,113  | 2.48 | 30 (36%) |
| 22  | CLA  | d     | 6004 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 25  | BCR  | K     | 1051 | -    | 41,41,41     | 4.03 | 17 (41%) | 56,56,56    | 4.97 | 20 (35%) |
| 25  | BCR  | T     | 6048 | -    | 41,41,41     | 4.01 | 17 (41%) | 56,56,56    | 6.30 | 27 (48%) |
| 22  | CLA  | c     | 6030 | -    | 69,73,73     | 1.91 | 17 (24%) | 82,113,113  | 2.48 | 29 (35%) |
| 22  | CLA  | A     | 1003 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | b     | 6019 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 28  | MGE  | d     | 6062 | -    | 48,48,48     | 0.97 | 2 (4%)   | 56,56,56    | 1.02 | 3 (5%)   |
| 22  | CLA  | b     | 6012 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | B     | 1014 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | c     | 6028 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.47 | 28 (34%) |
| 22  | CLA  | C     | 1033 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | h     | 6017 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | C     | 1027 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | b     | 6010 | 2    | 69,73,73     | 1.91 | 16 (23%) | 82,113,113  | 2.49 | 29 (35%) |
| 25  | BCR  | a     | 6044 | -    | 41,41,41     | 3.92 | 16 (39%) | 56,56,56    | 7.23 | 28 (50%) |
| 22  | CLA  | B     | 1023 | -    | 69,73,73     | 1.91 | 16 (23%) | 82,113,113  | 2.48 | 29 (35%) |
| 22  | CLA  | d     | 6008 | -    | 69,73,73     | 1.92 | 18 (26%) | 82,113,113  | 2.48 | 29 (35%) |
| 25  | BCR  | Z     | 1053 | -    | 41,41,41     | 4.03 | 17 (41%) | 56,56,56    | 6.02 | 21 (37%) |
| 29  | DGD  | B     | 1058 | -    | 67,67,67     | 0.86 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 22  | CLA  | c     | 6033 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.47 | 28 (34%) |
| 25  | BCR  | D     | 1050 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 5.17 | 22 (39%) |
| 25  | BCR  | B     | 1048 | -    | 41,41,41     | 4.01 | 17 (41%) | 56,56,56    | 6.30 | 27 (48%) |
| 22  | CLA  | c     | 6032 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.47 | 28 (34%) |
| 22  | CLA  | D     | 1004 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | a     | 6007 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | C     | 1025 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 31  | HEM  | f     | 6040 | 5    | 50,50,50     | 1.87 | 9 (18%)  | 67,82,82    | 1.34 | 5 (7%)   |
| 22  | CLA  | B     | 1010 | 2    | 69,73,73     | 1.92 | 16 (23%) | 82,113,113  | 2.49 | 29 (35%) |
| 22  | CLA  | K     | 1034 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 29  | DGD  | C     | 1056 | -    | 67,67,67     | 0.85 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 24  | PQ9  | d     | 6042 | -    | 45,45,45     | 0.68 | 2 (4%)   | 56,57,57    | 1.79 | 17 (30%) |
| 22  | CLA  | c     | 6027 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | b     | 6023 | -    | 69,73,73     | 1.91 | 16 (23%) | 82,113,113  | 2.48 | 29 (35%) |
| 22  | CLA  | C     | 1036 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | C     | 1028 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.47 | 27 (32%) |
| 22  | CLA  | b     | 6022 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | d     | 6005 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | B     | 1011 | -    | 69,73,73     | 1.92 | 16 (23%) | 82,113,113  | 2.47 | 30 (36%) |
| 22  | CLA  | C     | 1029 | -    | 69,73,73     | 1.91 | 17 (24%) | 82,113,113  | 2.48 | 29 (35%) |
| 25  | BCR  | A     | 1044 | -    | 41,41,41     | 3.93 | 16 (39%) | 56,56,56    | 7.23 | 28 (50%) |
| 22  | CLA  | C     | 1030 | -    | 69,73,73     | 1.91 | 17 (24%) | 82,113,113  | 2.48 | 29 (35%) |
| 22  | CLA  | C     | 1035 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 25  | BCR  | b     | 6047 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 5.46 | 27 (48%) |
| 23  | PHO  | d     | 6039 | -    | 58,69,69     | 2.94 | 13 (22%) | 55,99,99    | 3.52 | 19 (34%) |
| 22  | CLA  | c     | 6037 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | c     | 6025 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | LHG  | a     | 6063 | -    | 48,48,48     | 0.95 | 2 (4%)   | 51,54,54    | 1.05 | 3 (5%)   |
| 25  | BCR  | k     | 6051 | -    | 41,41,41     | 4.03 | 17 (41%) | 56,56,56    | 4.97 | 20 (35%) |
| 31  | HEM  | V     | 1041 | 16   | 50,50,50     | 1.88 | 8 (16%)  | 67,82,82    | 1.35 | 5 (7%)   |
| 22  | CLA  | b     | 6013 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 25  | BCR  | B     | 1045 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 6.17 | 21 (37%) |
| 22  | CLA  | b     | 6021 | 2    | 69,73,73     | 1.92 | 16 (23%) | 82,113,113  | 2.49 | 30 (36%) |
| 22  | CLA  | b     | 6018 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | A     | 1007 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | B     | 1012 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | b     | 6015 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | C     | 1037 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | B     | 1024 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 28  | MGE  | b     | 6060 | -    | 48,48,48     | 0.96 | 2 (4%)   | 56,56,56    | 1.02 | 3 (5%)   |
| 22  | CLA  | B     | 1019 | -    | 69,73,73     | 1.93 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 25  | BCR  | B     | 1047 | -    | 41,41,41     | 4.01 | 17 (41%) | 56,56,56    | 5.46 | 26 (46%) |
| 29  | DGD  | c     | 6055 | -    | 67,67,67     | 0.86 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 25  | BCR  | T     | 6046 | -    | 41,41,41     | 3.96 | 17 (41%) | 56,56,56    | 6.06 | 26 (46%) |
| 22  | CLA  | b     | 6009 | -    | 69,73,73     | 1.91 | 15 (21%) | 82,113,113  | 2.47 | 29 (35%) |
| 25  | BCR  | h     | 6049 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 5.30 | 20 (35%) |
| 25  | BCR  | H     | 1049 | -    | 41,41,41     | 4.02 | 16 (39%) | 56,56,56    | 5.30 | 20 (35%) |
| 28  | MGE  | L     | 1061 | -    | 48,48,48     | 0.96 | 2 (4%)   | 56,56,56    | 1.02 | 3 (5%)   |
| 29  | DGD  | c     | 6057 | -    | 67,67,67     | 0.86 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 28  | MGE  | B     | 1060 | -    | 48,48,48     | 0.96 | 2 (4%)   | 56,56,56    | 1.02 | 3 (5%)   |
| 22  | CLA  | c     | 6031 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 25  | BCR  | c     | 6054 | -    | 41,41,41     | 4.02 | 16 (39%) | 56,56,56    | 5.43 | 21 (37%) |
| 25  | BCR  | C     | 1054 | -    | 41,41,41     | 4.02 | 16 (39%) | 56,56,56    | 5.42 | 21 (37%) |
| 29  | DGD  | b     | 6058 | -    | 67,67,67     | 0.86 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 22  | CLA  | H     | 1017 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 29  | DGD  | C     | 1055 | -    | 67,67,67     | 0.86 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 22  | CLA  | b     | 6020 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.49 | 28 (34%) |
| 28  | MGE  | d     | 6059 | -    | 48,48,48     | 0.97 | 2 (4%)   | 56,56,56    | 1.01 | 3 (5%)   |
| 22  | CLA  | c     | 6036 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | b     | 6016 | -    | 69,73,73     | 1.93 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 28  | MGE  | D     | 1059 | -    | 48,48,48     | 0.97 | 2 (4%)   | 56,56,56    | 1.02 | 3 (5%)   |
| 25  | BCR  | z     | 6053 | -    | 41,41,41     | 4.03 | 17 (41%) | 56,56,56    | 6.02 | 22 (39%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | MGE  | l     | 6061 | -    | 48,48,48     | 0.96 | 2 (4%)   | 56,56,56    | 1.02 | 3 (5%)   |
| 29  | DGD  | C     | 1057 | -    | 67,67,67     | 0.85 | 2 (2%)   | 81,81,81    | 0.91 | 3 (3%)   |
| 24  | PQ9  | A     | 1043 | -    | 45,45,45     | 0.68 | 2 (4%)   | 56,57,57    | 1.79 | 17 (30%) |
| 22  | CLA  | B     | 1009 | -    | 69,73,73     | 1.92 | 15 (21%) | 82,113,113  | 2.47 | 29 (35%) |
| 25  | BCR  | d     | 6050 | -    | 41,41,41     | 4.02 | 17 (41%) | 56,56,56    | 5.17 | 21 (37%) |
| 22  | CLA  | B     | 1022 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.48 | 28 (34%) |
| 31  | HEM  | F     | 1040 | 5    | 50,50,50     | 1.87 | 8 (16%)  | 67,82,82    | 1.34 | 5 (7%)   |
| 22  | CLA  | C     | 1026 | -    | 69,73,73     | 1.94 | 15 (21%) | 82,113,113  | 2.48 | 28 (34%) |
| 22  | CLA  | c     | 6035 | -    | 69,73,73     | 1.94 | 16 (23%) | 82,113,113  | 2.49 | 28 (34%) |
| 23  | PHO  | D     | 1039 | -    | 58,69,69     | 2.94 | 13 (22%) | 55,99,99    | 3.52 | 19 (34%) |
| 24  | PQ9  | a     | 6043 | -    | 45,45,45     | 0.69 | 2 (4%)   | 56,57,57    | 1.79 | 17 (30%) |
| 22  | CLA  | c     | 6029 | -    | 69,73,73     | 1.91 | 16 (23%) | 82,113,113  | 2.48 | 29 (35%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | a     | 6003 | -    | 2/2/15/20 | 23/39/115/115 | -       |
| 23  | PHO  | a     | 6038 | -    | 1/1/17/22 | 18/37/103/103 | 0/5/6/6 |
| 22  | CLA  | B     | 1013 | -    | 2/2/15/20 | 24/39/115/115 | -       |
| 24  | PQ9  | D     | 1042 | -    | -         | 11/41/61/61   | 0/1/1/1 |
| 22  | CLA  | c     | 6026 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | A     | 1006 | -    | 2/2/15/20 | 19/39/115/115 | -       |
| 29  | DGD  | c     | 6056 | -    | -         | 32/55/95/95   | 0/2/2/2 |
| 22  | CLA  | b     | 6014 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 31  | HEM  | v     | 6041 | 16   | -         | 5/14/54/54    | -       |
| 25  | BCR  | t     | 1046 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 22  | CLA  | a     | 6006 | -    | 2/2/15/20 | 19/39/115/115 | -       |
| 23  | PHO  | A     | 1038 | -    | 1/1/17/22 | 18/37/103/103 | 0/5/6/6 |
| 22  | CLA  | D     | 1005 | -    | 2/2/15/20 | 20/39/115/115 | -       |
| 28  | MGE  | D     | 1062 | -    | -         | 24/43/63/63   | 0/1/1/1 |
| 25  | BCR  | b     | 6045 | -    | -         | 20/29/63/63   | 0/2/2/2 |
| 25  | BCR  | k     | 6052 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 1020 | -    | 3/3/15/20 | 18/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | D     | 1008 | -    | 3/3/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | B     | 1015 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | C     | 1031 | -    | 2/2/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | B     | 1016 | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 22  | CLA  | C     | 1032 | -    | 3/3/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | k     | 6034 | -    | 5/5/15/20 | 24/39/115/115 | -       |
| 25  | BCR  | C     | 1052 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 1018 | -    | 2/2/15/20 | 23/39/115/115 | -       |
| 22  | CLA  | B     | 1021 | 2    | 2/2/15/20 | 24/39/115/115 | -       |
| 26  | LHG  | A     | 1063 | -    | -         | 27/53/53/53   | -       |
| 22  | CLA  | b     | 6024 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | b     | 6011 | -    | 3/3/15/20 | 21/39/115/115 | -       |
| 22  | CLA  | d     | 6004 | -    | 2/2/15/20 | 12/39/115/115 | -       |
| 25  | BCR  | K     | 1051 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 25  | BCR  | T     | 6048 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 22  | CLA  | c     | 6030 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | A     | 1003 | -    | 2/2/15/20 | 23/39/115/115 | -       |
| 22  | CLA  | b     | 6019 | -    | 2/2/15/20 | 19/39/115/115 | -       |
| 28  | MGE  | d     | 6062 | -    | -         | 24/43/63/63   | 0/1/1/1 |
| 22  | CLA  | b     | 6012 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | B     | 1014 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | c     | 6028 | -    | 2/2/15/20 | 24/39/115/115 | -       |
| 22  | CLA  | C     | 1033 | -    | 2/2/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | h     | 6017 | -    | 2/2/15/20 | 24/39/115/115 | -       |
| 22  | CLA  | C     | 1027 | -    | 3/3/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | b     | 6010 | 2    | 2/2/15/20 | 15/39/115/115 | -       |
| 25  | BCR  | a     | 6044 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 1023 | -    | 3/3/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | d     | 6008 | -    | 3/3/15/20 | 15/39/115/115 | -       |
| 25  | BCR  | Z     | 1053 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 29  | DGD  | B     | 1058 | -    | -         | 32/55/95/95   | 0/2/2/2 |
| 22  | CLA  | c     | 6033 | -    | 2/2/15/20 | 16/39/115/115 | -       |
| 25  | BCR  | D     | 1050 | -    | -         | 21/29/63/63   | 0/2/2/2 |
| 25  | BCR  | B     | 1048 | -    | -         | 10/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | c     | 6032 | -    | 3/3/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | D     | 1004 | -    | 2/2/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | a     | 6007 | -    | 1/1/15/20 | 25/39/115/115 | -       |
| 22  | CLA  | C     | 1025 | -    | 2/2/15/20 | 17/39/115/115 | -       |
| 31  | HEM  | f     | 6040 | 5    | -         | 10/14/54/54   | -       |
| 22  | CLA  | B     | 1010 | 2    | 2/2/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | K     | 1034 | -    | 5/5/15/20 | 24/39/115/115 | -       |
| 29  | DGD  | C     | 1056 | -    | -         | 32/55/95/95   | 0/2/2/2 |
| 24  | PQ9  | d     | 6042 | -    | -         | 11/41/61/61   | 0/1/1/1 |
| 22  | CLA  | c     | 6027 | -    | 3/3/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | b     | 6023 | -    | 3/3/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | C     | 1036 | -    | 2/2/15/20 | 23/39/115/115 | -       |
| 22  | CLA  | C     | 1028 | -    | 2/2/15/20 | 24/39/115/115 | -       |
| 22  | CLA  | b     | 6022 | -    | 3/3/15/20 | 20/39/115/115 | -       |
| 22  | CLA  | d     | 6005 | -    | 2/2/15/20 | 20/39/115/115 | -       |
| 22  | CLA  | B     | 1011 | -    | 3/3/15/20 | 21/39/115/115 | -       |
| 22  | CLA  | C     | 1029 | -    | 3/3/15/20 | 15/39/115/115 | -       |
| 25  | BCR  | A     | 1044 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 22  | CLA  | C     | 1030 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | C     | 1035 | -    | 2/2/15/20 | 14/39/115/115 | -       |
| 25  | BCR  | b     | 6047 | -    | -         | 17/29/63/63   | 0/2/2/2 |
| 23  | PHO  | d     | 6039 | -    | 3/3/17/22 | 16/37/103/103 | 0/5/6/6 |
| 22  | CLA  | c     | 6037 | -    | 2/2/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | c     | 6025 | -    | 2/2/15/20 | 17/39/115/115 | -       |
| 26  | LHG  | a     | 6063 | -    | -         | 28/53/53/53   | -       |
| 25  | BCR  | k     | 6051 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 31  | HEM  | V     | 1041 | 16   | -         | 6/14/54/54    | -       |
| 22  | CLA  | b     | 6013 | -    | 2/2/15/20 | 24/39/115/115 | -       |
| 25  | BCR  | B     | 1045 | -    | -         | 20/29/63/63   | 0/2/2/2 |
| 22  | CLA  | b     | 6021 | 2    | 2/2/15/20 | 24/39/115/115 | -       |
| 22  | CLA  | b     | 6018 | -    | 2/2/15/20 | 23/39/115/115 | -       |
| 22  | CLA  | A     | 1007 | -    | 1/1/15/20 | 25/39/115/115 | -       |
| 22  | CLA  | B     | 1012 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | b     | 6015 | -    | 2/2/15/20 | 18/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | C     | 1037 | -    | 2/2/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | B     | 1024 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 28  | MGE  | b     | 6060 | -    | -         | 31/43/63/63   | 0/1/1/1 |
| 22  | CLA  | B     | 1019 | -    | 2/2/15/20 | 19/39/115/115 | -       |
| 25  | BCR  | B     | 1047 | -    | -         | 17/29/63/63   | 0/2/2/2 |
| 29  | DGD  | c     | 6055 | -    | -         | 33/55/95/95   | 0/2/2/2 |
| 25  | BCR  | T     | 6046 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 22  | CLA  | b     | 6009 | -    | 2/2/15/20 | 17/39/115/115 | -       |
| 25  | BCR  | h     | 6049 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 25  | BCR  | H     | 1049 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 28  | MGE  | L     | 1061 | -    | -         | 26/43/63/63   | 0/1/1/1 |
| 29  | DGD  | c     | 6057 | -    | -         | 32/55/95/95   | 0/2/2/2 |
| 28  | MGE  | B     | 1060 | -    | -         | 31/43/63/63   | 0/1/1/1 |
| 22  | CLA  | c     | 6031 | -    | 2/2/15/20 | 14/39/115/115 | -       |
| 25  | BCR  | c     | 6054 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 25  | BCR  | C     | 1054 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 29  | DGD  | b     | 6058 | -    | -         | 32/55/95/95   | 0/2/2/2 |
| 22  | CLA  | H     | 1017 | -    | 2/2/15/20 | 24/39/115/115 | -       |
| 29  | DGD  | C     | 1055 | -    | -         | 33/55/95/95   | 0/2/2/2 |
| 22  | CLA  | b     | 6020 | -    | 3/3/15/20 | 18/39/115/115 | -       |
| 28  | MGE  | d     | 6059 | -    | -         | 23/43/63/63   | 0/1/1/1 |
| 22  | CLA  | c     | 6036 | -    | 2/2/15/20 | 23/39/115/115 | -       |
| 22  | CLA  | b     | 6016 | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 28  | MGE  | D     | 1059 | -    | -         | 23/43/63/63   | 0/1/1/1 |
| 25  | BCR  | z     | 6053 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 28  | MGE  | l     | 6061 | -    | -         | 26/43/63/63   | 0/1/1/1 |
| 29  | DGD  | C     | 1057 | -    | -         | 32/55/95/95   | 0/2/2/2 |
| 24  | PQ9  | A     | 1043 | -    | -         | 16/41/61/61   | 0/1/1/1 |
| 22  | CLA  | B     | 1009 | -    | 2/2/15/20 | 17/39/115/115 | -       |
| 25  | BCR  | d     | 6050 | -    | -         | 21/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 1022 | -    | 3/3/15/20 | 20/39/115/115 | -       |
| 31  | HEM  | F     | 1040 | 5    | -         | 10/14/54/54   | -       |
| 22  | CLA  | C     | 1026 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | c     | 6035 | -    | 2/2/15/20 | 14/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 23  | PHO  | D     | 1039 | -    | 3/3/17/22 | 16/37/103/103 | 0/5/6/6 |
| 24  | PQ9  | a     | 6043 | -    | -         | 16/41/61/61   | 0/1/1/1 |
| 22  | CLA  | c     | 6029 | -    | 3/3/15/20 | 15/39/115/115 | -       |

All (1605) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | d     | 6039 | PHO  | OBD-CAD | 14.60 | 1.41        | 1.22     |
| 23  | D     | 1039 | PHO  | OBD-CAD | 14.58 | 1.41        | 1.22     |
| 23  | A     | 1038 | PHO  | OBD-CAD | 14.57 | 1.41        | 1.22     |
| 23  | a     | 6038 | PHO  | OBD-CAD | 14.57 | 1.41        | 1.22     |
| 25  | b     | 6047 | BCR  | C19-C18 | -9.39 | 1.25        | 1.46     |
| 25  | z     | 6053 | BCR  | C8-C9   | -9.39 | 1.25        | 1.46     |
| 25  | b     | 6047 | BCR  | C8-C9   | -9.38 | 1.25        | 1.46     |
| 25  | k     | 6051 | BCR  | C12-C13 | -9.38 | 1.25        | 1.46     |
| 25  | B     | 1047 | BCR  | C8-C9   | -9.38 | 1.25        | 1.46     |
| 25  | c     | 6054 | BCR  | C8-C9   | -9.38 | 1.25        | 1.46     |
| 25  | C     | 1054 | BCR  | C8-C9   | -9.37 | 1.25        | 1.46     |
| 25  | B     | 1047 | BCR  | C19-C18 | -9.37 | 1.25        | 1.46     |
| 25  | Z     | 1053 | BCR  | C8-C9   | -9.37 | 1.25        | 1.46     |
| 25  | k     | 6052 | BCR  | C12-C13 | -9.37 | 1.25        | 1.46     |
| 25  | h     | 6049 | BCR  | C19-C18 | -9.37 | 1.25        | 1.46     |
| 25  | B     | 1048 | BCR  | C8-C9   | -9.37 | 1.25        | 1.46     |
| 25  | K     | 1051 | BCR  | C12-C13 | -9.37 | 1.25        | 1.46     |
| 25  | C     | 1052 | BCR  | C12-C13 | -9.36 | 1.25        | 1.46     |
| 25  | B     | 1045 | BCR  | C19-C18 | -9.36 | 1.25        | 1.46     |
| 25  | T     | 6048 | BCR  | C8-C9   | -9.36 | 1.25        | 1.46     |
| 25  | H     | 1049 | BCR  | C19-C18 | -9.36 | 1.25        | 1.46     |
| 25  | B     | 1045 | BCR  | C8-C9   | -9.36 | 1.25        | 1.46     |
| 25  | Z     | 1053 | BCR  | C12-C13 | -9.36 | 1.25        | 1.46     |
| 25  | B     | 1048 | BCR  | C12-C13 | -9.35 | 1.25        | 1.46     |
| 25  | k     | 6051 | BCR  | C8-C9   | -9.35 | 1.25        | 1.46     |
| 25  | b     | 6045 | BCR  | C19-C18 | -9.35 | 1.25        | 1.46     |
| 25  | D     | 1050 | BCR  | C12-C13 | -9.35 | 1.25        | 1.46     |
| 25  | C     | 1054 | BCR  | C19-C18 | -9.35 | 1.25        | 1.46     |
| 25  | T     | 6048 | BCR  | C12-C13 | -9.35 | 1.25        | 1.46     |
| 25  | b     | 6045 | BCR  | C8-C9   | -9.35 | 1.25        | 1.46     |
| 25  | z     | 6053 | BCR  | C12-C13 | -9.35 | 1.26        | 1.46     |
| 25  | D     | 1050 | BCR  | C19-C18 | -9.34 | 1.26        | 1.46     |
| 25  | K     | 1051 | BCR  | C8-C9   | -9.34 | 1.26        | 1.46     |
| 25  | h     | 6049 | BCR  | C12-C13 | -9.34 | 1.26        | 1.46     |
| 25  | z     | 6053 | BCR  | C19-C18 | -9.34 | 1.26        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | H     | 1049 | BCR  | C12-C13 | -9.33 | 1.26        | 1.46     |
| 25  | k     | 6052 | BCR  | C8-C9   | -9.33 | 1.26        | 1.46     |
| 25  | K     | 1051 | BCR  | C19-C18 | -9.33 | 1.26        | 1.46     |
| 25  | c     | 6054 | BCR  | C19-C18 | -9.33 | 1.26        | 1.46     |
| 25  | B     | 1047 | BCR  | C12-C13 | -9.33 | 1.26        | 1.46     |
| 25  | c     | 6054 | BCR  | C12-C13 | -9.33 | 1.26        | 1.46     |
| 25  | C     | 1052 | BCR  | C19-C18 | -9.33 | 1.26        | 1.46     |
| 25  | Z     | 1053 | BCR  | C19-C18 | -9.33 | 1.26        | 1.46     |
| 25  | C     | 1054 | BCR  | C12-C13 | -9.33 | 1.26        | 1.46     |
| 25  | d     | 6050 | BCR  | C12-C13 | -9.33 | 1.26        | 1.46     |
| 25  | d     | 6050 | BCR  | C19-C18 | -9.33 | 1.26        | 1.46     |
| 25  | k     | 6052 | BCR  | C19-C18 | -9.32 | 1.26        | 1.46     |
| 25  | h     | 6049 | BCR  | C8-C9   | -9.32 | 1.26        | 1.46     |
| 25  | C     | 1052 | BCR  | C8-C9   | -9.32 | 1.26        | 1.46     |
| 25  | b     | 6045 | BCR  | C12-C13 | -9.32 | 1.26        | 1.46     |
| 25  | k     | 6051 | BCR  | C19-C18 | -9.32 | 1.26        | 1.46     |
| 25  | H     | 1049 | BCR  | C8-C9   | -9.32 | 1.26        | 1.46     |
| 25  | b     | 6047 | BCR  | C12-C13 | -9.32 | 1.26        | 1.46     |
| 25  | B     | 1045 | BCR  | C12-C13 | -9.31 | 1.26        | 1.46     |
| 25  | B     | 1048 | BCR  | C19-C18 | -9.31 | 1.26        | 1.46     |
| 25  | T     | 6048 | BCR  | C19-C18 | -9.31 | 1.26        | 1.46     |
| 25  | D     | 1050 | BCR  | C8-C9   | -9.30 | 1.26        | 1.46     |
| 25  | d     | 6050 | BCR  | C8-C9   | -9.30 | 1.26        | 1.46     |
| 25  | a     | 6044 | BCR  | C19-C18 | -9.27 | 1.26        | 1.46     |
| 25  | T     | 6046 | BCR  | C12-C13 | -9.27 | 1.26        | 1.46     |
| 25  | A     | 1044 | BCR  | C19-C18 | -9.26 | 1.26        | 1.46     |
| 25  | t     | 1046 | BCR  | C12-C13 | -9.26 | 1.26        | 1.46     |
| 25  | t     | 1046 | BCR  | C8-C9   | -9.23 | 1.26        | 1.46     |
| 25  | T     | 6046 | BCR  | C8-C9   | -9.21 | 1.26        | 1.46     |
| 25  | T     | 6046 | BCR  | C19-C18 | -9.20 | 1.26        | 1.46     |
| 25  | t     | 1046 | BCR  | C19-C18 | -9.19 | 1.26        | 1.46     |
| 25  | A     | 1044 | BCR  | C8-C9   | -9.13 | 1.26        | 1.46     |
| 25  | a     | 6044 | BCR  | C8-C9   | -9.12 | 1.26        | 1.46     |
| 25  | A     | 1044 | BCR  | C12-C13 | -9.06 | 1.26        | 1.46     |
| 25  | a     | 6044 | BCR  | C12-C13 | -9.06 | 1.26        | 1.46     |
| 23  | a     | 6038 | PHO  | O1D-CGD | 8.05  | 1.41        | 1.21     |
| 23  | D     | 1039 | PHO  | O1D-CGD | 8.03  | 1.41        | 1.21     |
| 23  | A     | 1038 | PHO  | O1D-CGD | 8.03  | 1.41        | 1.21     |
| 25  | c     | 6054 | BCR  | C16-C17 | -8.02 | 1.18        | 1.43     |
| 25  | b     | 6047 | BCR  | C16-C17 | -8.01 | 1.18        | 1.43     |
| 23  | d     | 6039 | PHO  | O1D-CGD | 8.01  | 1.41        | 1.21     |
| 25  | C     | 1054 | BCR  | C16-C17 | -8.01 | 1.18        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | b     | 6047 | BCR  | C20-C21 | -8.00 | 1.18        | 1.43     |
| 25  | H     | 1049 | BCR  | C20-C21 | -8.00 | 1.18        | 1.43     |
| 25  | h     | 6049 | BCR  | C20-C21 | -7.99 | 1.18        | 1.43     |
| 25  | B     | 1048 | BCR  | C20-C21 | -7.99 | 1.18        | 1.43     |
| 25  | B     | 1047 | BCR  | C16-C17 | -7.99 | 1.18        | 1.43     |
| 25  | Z     | 1053 | BCR  | C16-C17 | -7.99 | 1.18        | 1.43     |
| 25  | B     | 1045 | BCR  | C16-C17 | -7.99 | 1.18        | 1.43     |
| 25  | K     | 1051 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | b     | 6045 | BCR  | C16-C17 | -7.98 | 1.18        | 1.43     |
| 25  | k     | 6051 | BCR  | C16-C17 | -7.98 | 1.18        | 1.43     |
| 25  | B     | 1047 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | C     | 1052 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | K     | 1051 | BCR  | C16-C17 | -7.98 | 1.18        | 1.43     |
| 25  | b     | 6045 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | C     | 1054 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | z     | 6053 | BCR  | C16-C17 | -7.98 | 1.18        | 1.43     |
| 25  | B     | 1045 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | c     | 6054 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | k     | 6051 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 25  | z     | 6053 | BCR  | C20-C21 | -7.97 | 1.18        | 1.43     |
| 25  | d     | 6050 | BCR  | C16-C17 | -7.97 | 1.18        | 1.43     |
| 25  | H     | 1049 | BCR  | C16-C17 | -7.97 | 1.18        | 1.43     |
| 25  | T     | 6048 | BCR  | C16-C17 | -7.97 | 1.18        | 1.43     |
| 25  | k     | 6052 | BCR  | C20-C21 | -7.97 | 1.18        | 1.43     |
| 25  | C     | 1052 | BCR  | C16-C17 | -7.97 | 1.18        | 1.43     |
| 25  | D     | 1050 | BCR  | C16-C17 | -7.97 | 1.18        | 1.43     |
| 25  | Z     | 1053 | BCR  | C20-C21 | -7.97 | 1.18        | 1.43     |
| 25  | T     | 6048 | BCR  | C20-C21 | -7.97 | 1.18        | 1.43     |
| 25  | d     | 6050 | BCR  | C20-C21 | -7.96 | 1.18        | 1.43     |
| 25  | h     | 6049 | BCR  | C16-C17 | -7.96 | 1.18        | 1.43     |
| 25  | D     | 1050 | BCR  | C20-C21 | -7.96 | 1.18        | 1.43     |
| 25  | B     | 1048 | BCR  | C16-C17 | -7.95 | 1.18        | 1.43     |
| 31  | V     | 1041 | HEM  | C3D-C2D | 7.95  | 1.53        | 1.36     |
| 25  | k     | 6052 | BCR  | C16-C17 | -7.94 | 1.18        | 1.43     |
| 31  | v     | 6041 | HEM  | C3D-C2D | 7.92  | 1.53        | 1.36     |
| 31  | F     | 1040 | HEM  | C3D-C2D | 7.89  | 1.53        | 1.36     |
| 25  | T     | 6046 | BCR  | C16-C17 | -7.86 | 1.18        | 1.43     |
| 25  | t     | 1046 | BCR  | C16-C17 | -7.86 | 1.18        | 1.43     |
| 31  | f     | 6040 | HEM  | C3D-C2D | 7.86  | 1.53        | 1.36     |
| 25  | a     | 6044 | BCR  | C20-C21 | -7.86 | 1.18        | 1.43     |
| 25  | A     | 1044 | BCR  | C20-C21 | -7.84 | 1.18        | 1.43     |
| 25  | a     | 6044 | BCR  | C16-C17 | -7.83 | 1.18        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | A     | 1044 | BCR  | C16-C17 | -7.82 | 1.18        | 1.43     |
| 25  | t     | 1046 | BCR  | C20-C21 | -7.77 | 1.19        | 1.43     |
| 25  | T     | 6046 | BCR  | C20-C21 | -7.76 | 1.19        | 1.43     |
| 25  | h     | 6049 | BCR  | C16-C15 | -6.52 | 1.18        | 1.36     |
| 25  | k     | 6052 | BCR  | C16-C15 | -6.51 | 1.18        | 1.36     |
| 25  | K     | 1051 | BCR  | C16-C15 | -6.51 | 1.18        | 1.36     |
| 25  | H     | 1049 | BCR  | C16-C15 | -6.51 | 1.18        | 1.36     |
| 25  | k     | 6051 | BCR  | C16-C15 | -6.51 | 1.18        | 1.36     |
| 25  | z     | 6053 | BCR  | C16-C15 | -6.50 | 1.18        | 1.36     |
| 25  | C     | 1052 | BCR  | C16-C15 | -6.50 | 1.18        | 1.36     |
| 25  | Z     | 1053 | BCR  | C16-C15 | -6.49 | 1.18        | 1.36     |
| 25  | B     | 1048 | BCR  | C16-C15 | -6.49 | 1.18        | 1.36     |
| 25  | b     | 6047 | BCR  | C16-C15 | -6.48 | 1.18        | 1.36     |
| 25  | B     | 1047 | BCR  | C16-C15 | -6.48 | 1.18        | 1.36     |
| 25  | C     | 1054 | BCR  | C16-C15 | -6.47 | 1.18        | 1.36     |
| 25  | B     | 1045 | BCR  | C16-C15 | -6.47 | 1.18        | 1.36     |
| 25  | T     | 6048 | BCR  | C16-C15 | -6.47 | 1.18        | 1.36     |
| 25  | b     | 6045 | BCR  | C16-C15 | -6.46 | 1.18        | 1.36     |
| 25  | D     | 1050 | BCR  | C16-C15 | -6.46 | 1.18        | 1.36     |
| 25  | d     | 6050 | BCR  | C16-C15 | -6.46 | 1.18        | 1.36     |
| 25  | c     | 6054 | BCR  | C16-C15 | -6.45 | 1.18        | 1.36     |
| 23  | A     | 1038 | PHO  | O1A-CGA | 6.36  | 1.41        | 1.22     |
| 23  | d     | 6039 | PHO  | O1A-CGA | 6.35  | 1.41        | 1.22     |
| 23  | D     | 1039 | PHO  | O1A-CGA | 6.35  | 1.41        | 1.22     |
| 23  | a     | 6038 | PHO  | O1A-CGA | 6.34  | 1.41        | 1.22     |
| 25  | t     | 1046 | BCR  | C16-C15 | -6.31 | 1.18        | 1.36     |
| 25  | T     | 6046 | BCR  | C16-C15 | -6.31 | 1.18        | 1.36     |
| 23  | d     | 6039 | PHO  | C2-C3   | 6.27  | 1.47        | 1.33     |
| 23  | D     | 1039 | PHO  | C2-C3   | 6.26  | 1.47        | 1.33     |
| 25  | b     | 6047 | BCR  | C11-C12 | -6.25 | 1.18        | 1.34     |
| 25  | c     | 6054 | BCR  | C20-C19 | -6.25 | 1.18        | 1.34     |
| 25  | T     | 6048 | BCR  | C20-C19 | -6.24 | 1.18        | 1.34     |
| 25  | k     | 6051 | BCR  | C20-C19 | -6.24 | 1.18        | 1.34     |
| 25  | d     | 6050 | BCR  | C20-C19 | -6.24 | 1.18        | 1.34     |
| 25  | a     | 6044 | BCR  | C16-C15 | -6.24 | 1.19        | 1.36     |
| 23  | A     | 1038 | PHO  | C2-C3   | 6.24  | 1.47        | 1.33     |
| 25  | C     | 1054 | BCR  | C11-C12 | -6.24 | 1.18        | 1.34     |
| 23  | a     | 6038 | PHO  | C2-C3   | 6.24  | 1.47        | 1.33     |
| 25  | B     | 1048 | BCR  | C20-C19 | -6.24 | 1.18        | 1.34     |
| 25  | z     | 6053 | BCR  | C11-C12 | -6.23 | 1.18        | 1.34     |
| 25  | k     | 6052 | BCR  | C20-C19 | -6.23 | 1.18        | 1.34     |
| 25  | B     | 1047 | BCR  | C11-C12 | -6.23 | 1.18        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | b     | 6045 | BCR  | C11-C12 | -6.23 | 1.18        | 1.34     |
| 25  | A     | 1044 | BCR  | C16-C15 | -6.22 | 1.19        | 1.36     |
| 25  | D     | 1050 | BCR  | C20-C19 | -6.22 | 1.18        | 1.34     |
| 25  | k     | 6052 | BCR  | C11-C12 | -6.22 | 1.18        | 1.34     |
| 25  | c     | 6054 | BCR  | C11-C12 | -6.22 | 1.18        | 1.34     |
| 25  | K     | 1051 | BCR  | C20-C19 | -6.22 | 1.18        | 1.34     |
| 25  | C     | 1054 | BCR  | C20-C19 | -6.22 | 1.18        | 1.34     |
| 25  | B     | 1045 | BCR  | C11-C12 | -6.22 | 1.18        | 1.34     |
| 25  | H     | 1049 | BCR  | C11-C12 | -6.22 | 1.18        | 1.34     |
| 25  | Z     | 1053 | BCR  | C11-C12 | -6.22 | 1.18        | 1.34     |
| 25  | B     | 1048 | BCR  | C11-C12 | -6.22 | 1.18        | 1.34     |
| 25  | C     | 1052 | BCR  | C20-C19 | -6.21 | 1.18        | 1.34     |
| 25  | B     | 1045 | BCR  | C20-C19 | -6.21 | 1.18        | 1.34     |
| 25  | h     | 6049 | BCR  | C20-C19 | -6.21 | 1.18        | 1.34     |
| 25  | B     | 1047 | BCR  | C20-C19 | -6.21 | 1.18        | 1.34     |
| 25  | K     | 1051 | BCR  | C11-C12 | -6.21 | 1.18        | 1.34     |
| 25  | h     | 6049 | BCR  | C11-C12 | -6.21 | 1.18        | 1.34     |
| 25  | T     | 6048 | BCR  | C11-C12 | -6.20 | 1.18        | 1.34     |
| 25  | C     | 1052 | BCR  | C11-C12 | -6.20 | 1.18        | 1.34     |
| 25  | d     | 6050 | BCR  | C11-C12 | -6.20 | 1.18        | 1.34     |
| 25  | b     | 6045 | BCR  | C20-C19 | -6.20 | 1.18        | 1.34     |
| 25  | H     | 1049 | BCR  | C20-C19 | -6.20 | 1.18        | 1.34     |
| 25  | Z     | 1053 | BCR  | C20-C19 | -6.20 | 1.18        | 1.34     |
| 25  | D     | 1050 | BCR  | C11-C12 | -6.19 | 1.18        | 1.34     |
| 25  | k     | 6051 | BCR  | C11-C12 | -6.19 | 1.18        | 1.34     |
| 25  | z     | 6053 | BCR  | C20-C19 | -6.19 | 1.18        | 1.34     |
| 25  | b     | 6047 | BCR  | C20-C19 | -6.18 | 1.18        | 1.34     |
| 25  | T     | 6046 | BCR  | C11-C12 | -6.05 | 1.18        | 1.34     |
| 25  | A     | 1044 | BCR  | C20-C19 | -6.05 | 1.18        | 1.34     |
| 25  | t     | 1046 | BCR  | C11-C12 | -6.04 | 1.18        | 1.34     |
| 25  | a     | 6044 | BCR  | C20-C19 | -6.03 | 1.18        | 1.34     |
| 25  | T     | 6046 | BCR  | C20-C19 | -6.02 | 1.19        | 1.34     |
| 25  | A     | 1044 | BCR  | C11-C12 | -6.02 | 1.19        | 1.34     |
| 25  | t     | 1046 | BCR  | C20-C19 | -6.01 | 1.19        | 1.34     |
| 25  | a     | 6044 | BCR  | C11-C12 | -6.01 | 1.19        | 1.34     |
| 25  | d     | 6050 | BCR  | C11-C10 | -5.58 | 1.25        | 1.43     |
| 25  | T     | 6048 | BCR  | C11-C10 | -5.58 | 1.25        | 1.43     |
| 25  | D     | 1050 | BCR  | C11-C10 | -5.57 | 1.25        | 1.43     |
| 25  | C     | 1052 | BCR  | C11-C10 | -5.57 | 1.25        | 1.43     |
| 25  | b     | 6047 | BCR  | C15-C14 | -5.57 | 1.25        | 1.43     |
| 25  | B     | 1045 | BCR  | C11-C10 | -5.56 | 1.25        | 1.43     |
| 25  | B     | 1047 | BCR  | C15-C14 | -5.56 | 1.25        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | h     | 6049 | BCR  | C11-C10 | -5.56 | 1.25        | 1.43     |
| 25  | B     | 1048 | BCR  | C15-C14 | -5.56 | 1.25        | 1.43     |
| 25  | B     | 1048 | BCR  | C11-C10 | -5.56 | 1.25        | 1.43     |
| 25  | k     | 6051 | BCR  | C11-C10 | -5.56 | 1.25        | 1.43     |
| 25  | D     | 1050 | BCR  | C15-C14 | -5.56 | 1.25        | 1.43     |
| 25  | b     | 6045 | BCR  | C11-C10 | -5.56 | 1.25        | 1.43     |
| 25  | d     | 6050 | BCR  | C15-C14 | -5.56 | 1.25        | 1.43     |
| 25  | H     | 1049 | BCR  | C11-C10 | -5.56 | 1.25        | 1.43     |
| 25  | k     | 6051 | BCR  | C15-C14 | -5.56 | 1.25        | 1.43     |
| 25  | B     | 1045 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | b     | 6045 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | K     | 1051 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | K     | 1051 | BCR  | C11-C10 | -5.55 | 1.26        | 1.43     |
| 25  | c     | 6054 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | z     | 6053 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | h     | 6049 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | H     | 1049 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | c     | 6054 | BCR  | C11-C10 | -5.55 | 1.26        | 1.43     |
| 25  | k     | 6052 | BCR  | C11-C10 | -5.55 | 1.26        | 1.43     |
| 25  | C     | 1054 | BCR  | C11-C10 | -5.55 | 1.26        | 1.43     |
| 25  | z     | 6053 | BCR  | C11-C10 | -5.55 | 1.26        | 1.43     |
| 25  | k     | 6052 | BCR  | C15-C14 | -5.55 | 1.26        | 1.43     |
| 25  | Z     | 1053 | BCR  | C11-C10 | -5.54 | 1.26        | 1.43     |
| 25  | Z     | 1053 | BCR  | C15-C14 | -5.54 | 1.26        | 1.43     |
| 25  | C     | 1054 | BCR  | C15-C14 | -5.54 | 1.26        | 1.43     |
| 25  | B     | 1047 | BCR  | C11-C10 | -5.54 | 1.26        | 1.43     |
| 25  | T     | 6048 | BCR  | C15-C14 | -5.54 | 1.26        | 1.43     |
| 25  | C     | 1052 | BCR  | C15-C14 | -5.54 | 1.26        | 1.43     |
| 25  | b     | 6047 | BCR  | C11-C10 | -5.53 | 1.26        | 1.43     |
| 25  | T     | 6046 | BCR  | C11-C10 | -5.50 | 1.26        | 1.43     |
| 25  | t     | 1046 | BCR  | C11-C10 | -5.48 | 1.26        | 1.43     |
| 25  | a     | 6044 | BCR  | C15-C14 | -5.42 | 1.26        | 1.43     |
| 25  | A     | 1044 | BCR  | C15-C14 | -5.41 | 1.26        | 1.43     |
| 25  | T     | 6046 | BCR  | C15-C14 | -5.41 | 1.26        | 1.43     |
| 25  | t     | 1046 | BCR  | C15-C14 | -5.41 | 1.26        | 1.43     |
| 25  | A     | 1044 | BCR  | C11-C10 | -5.39 | 1.26        | 1.43     |
| 25  | a     | 6044 | BCR  | C11-C10 | -5.39 | 1.26        | 1.43     |
| 25  | D     | 1050 | BCR  | C23-C22 | -5.39 | 1.34        | 1.46     |
| 25  | H     | 1049 | BCR  | C23-C22 | -5.38 | 1.34        | 1.46     |
| 25  | d     | 6050 | BCR  | C23-C22 | -5.38 | 1.34        | 1.46     |
| 25  | B     | 1045 | BCR  | C23-C22 | -5.38 | 1.34        | 1.46     |
| 25  | h     | 6049 | BCR  | C23-C22 | -5.38 | 1.34        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | b     | 6045 | BCR  | C23-C22 | -5.37 | 1.34        | 1.46     |
| 25  | c     | 6054 | BCR  | C23-C22 | -5.37 | 1.34        | 1.46     |
| 25  | C     | 1054 | BCR  | C23-C22 | -5.36 | 1.34        | 1.46     |
| 25  | K     | 1051 | BCR  | C23-C22 | -5.35 | 1.34        | 1.46     |
| 25  | z     | 6053 | BCR  | C23-C22 | -5.35 | 1.34        | 1.46     |
| 25  | Z     | 1053 | BCR  | C23-C22 | -5.35 | 1.34        | 1.46     |
| 25  | k     | 6051 | BCR  | C23-C22 | -5.31 | 1.34        | 1.46     |
| 25  | T     | 6046 | BCR  | C23-C22 | -5.28 | 1.34        | 1.46     |
| 25  | t     | 1046 | BCR  | C23-C22 | -5.27 | 1.34        | 1.46     |
| 22  | B     | 1011 | CLA  | O2D-CGD | 5.20  | 1.46        | 1.33     |
| 22  | b     | 6011 | CLA  | O2D-CGD | 5.19  | 1.46        | 1.33     |
| 22  | A     | 1007 | CLA  | O2D-CGD | 5.18  | 1.46        | 1.33     |
| 22  | b     | 6024 | CLA  | O2D-CGD | 5.18  | 1.46        | 1.33     |
| 22  | c     | 6032 | CLA  | O2D-CGD | 5.18  | 1.46        | 1.33     |
| 22  | C     | 1036 | CLA  | O2D-CGD | 5.17  | 1.45        | 1.33     |
| 22  | a     | 6007 | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 22  | c     | 6033 | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 22  | C     | 1033 | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 22  | b     | 6022 | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 25  | A     | 1044 | BCR  | C23-C22 | -5.16 | 1.34        | 1.46     |
| 22  | B     | 1024 | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 25  | a     | 6044 | BCR  | C23-C22 | -5.15 | 1.34        | 1.46     |
| 22  | C     | 1032 | CLA  | O2D-CGD | 5.15  | 1.45        | 1.33     |
| 22  | C     | 1025 | CLA  | O2D-CGD | 5.15  | 1.45        | 1.33     |
| 25  | C     | 1052 | BCR  | C23-C22 | -5.15 | 1.34        | 1.46     |
| 22  | C     | 1035 | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 22  | B     | 1013 | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 22  | b     | 6010 | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 22  | A     | 1006 | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 22  | C     | 1031 | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 22  | C     | 1027 | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 22  | c     | 6026 | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 22  | B     | 1020 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | c     | 6025 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | b     | 6012 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | b     | 6020 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | D     | 1004 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | b     | 6014 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 25  | k     | 6052 | BCR  | C23-C22 | -5.13 | 1.35        | 1.46     |
| 22  | B     | 1012 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | D     | 1005 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | B     | 1010 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | C     | 1028 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | c     | 6036 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | B     | 1019 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | C     | 1026 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | K     | 1034 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | B     | 1016 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | c     | 6027 | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 22  | B     | 1022 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | a     | 6003 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | b     | 6013 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | B     | 1018 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | H     | 1017 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | c     | 6028 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | d     | 6004 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | b     | 6016 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | h     | 6017 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | d     | 6005 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | b     | 6019 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | c     | 6037 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 22  | c     | 6035 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 25  | T     | 6048 | BCR  | C23-C22 | -5.11 | 1.35        | 1.46     |
| 22  | A     | 1003 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 22  | C     | 1037 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 22  | b     | 6018 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 22  | k     | 6034 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 22  | a     | 6006 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 22  | B     | 1014 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 22  | d     | 6008 | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 22  | c     | 6031 | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 22  | B     | 1015 | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 25  | B     | 1048 | BCR  | C23-C22 | -5.10 | 1.35        | 1.46     |
| 22  | D     | 1008 | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 22  | b     | 6015 | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 25  | B     | 1047 | BCR  | C23-C22 | -5.09 | 1.35        | 1.46     |
| 25  | b     | 6047 | BCR  | C23-C22 | -5.08 | 1.35        | 1.46     |
| 22  | b     | 6009 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 22  | B     | 1009 | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 22  | c     | 6029 | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 22  | C     | 1029 | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 22  | c     | 6030 | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 22  | C     | 1030 | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 22  | B     | 1023 | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | b     | 6023 | CLA  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 22  | B     | 1021 | CLA  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 22  | b     | 6021 | CLA  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 22  | a     | 6003 | CLA  | C3C-C2C | 4.87  | 1.47        | 1.36     |
| 22  | k     | 6034 | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 22  | b     | 6014 | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 22  | b     | 6015 | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 22  | K     | 1034 | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 22  | c     | 6027 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 22  | A     | 1003 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 22  | D     | 1004 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 22  | a     | 6007 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 22  | B     | 1014 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 23  | A     | 1038 | PHO  | C3D-C4D | -4.84 | 1.34        | 1.41     |
| 22  | a     | 6006 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 23  | d     | 6039 | PHO  | C3D-C4D | -4.84 | 1.34        | 1.41     |
| 22  | b     | 6011 | CLA  | C3D-C4D | -4.84 | 1.33        | 1.44     |
| 22  | h     | 6017 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 23  | D     | 1039 | PHO  | C3D-C4D | -4.84 | 1.34        | 1.41     |
| 22  | b     | 6018 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 22  | H     | 1017 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 22  | C     | 1027 | CLA  | C3C-C2C | 4.84  | 1.47        | 1.36     |
| 22  | c     | 6035 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | C     | 1025 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 23  | a     | 6038 | PHO  | C3D-C4D | -4.83 | 1.34        | 1.41     |
| 22  | B     | 1016 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | B     | 1024 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | d     | 6004 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | B     | 1018 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | b     | 6012 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | b     | 6020 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | c     | 6032 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |
| 22  | B     | 1013 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 22  | c     | 6030 | CLA  | C3D-C4D | -4.82 | 1.33        | 1.44     |
| 22  | A     | 1007 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 22  | C     | 1026 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 22  | B     | 1022 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 22  | c     | 6031 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 22  | B     | 1020 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 22  | C     | 1031 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 22  | d     | 6005 | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 23  | d     | 6039 | PHO  | C3D-C2D | 4.82  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1012 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | d     | 6008 | CLA  | C3D-C4D | -4.81 | 1.33        | 1.44     |
| 22  | B     | 1011 | CLA  | C3D-C4D | -4.81 | 1.33        | 1.44     |
| 22  | c     | 6029 | CLA  | C3D-C4D | -4.81 | 1.33        | 1.44     |
| 22  | B     | 1015 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | b     | 6016 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | C     | 1032 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | C     | 1036 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | A     | 1006 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | D     | 1008 | CLA  | C3D-C4D | -4.81 | 1.33        | 1.44     |
| 23  | A     | 1038 | PHO  | C3D-C2D | 4.81  | 1.47        | 1.39     |
| 22  | b     | 6021 | CLA  | C3D-C4D | -4.81 | 1.33        | 1.44     |
| 22  | C     | 1035 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | c     | 6025 | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 22  | C     | 1037 | CLA  | C3C-C2C | 4.80  | 1.47        | 1.36     |
| 22  | D     | 1005 | CLA  | C3C-C2C | 4.80  | 1.47        | 1.36     |
| 22  | c     | 6026 | CLA  | C3C-C2C | 4.80  | 1.47        | 1.36     |
| 22  | c     | 6028 | CLA  | C3C-C2C | 4.80  | 1.47        | 1.36     |
| 22  | B     | 1010 | CLA  | C3D-C4D | -4.80 | 1.33        | 1.44     |
| 22  | b     | 6013 | CLA  | C3C-C2C | 4.80  | 1.47        | 1.36     |
| 22  | b     | 6010 | CLA  | C3D-C4D | -4.80 | 1.33        | 1.44     |
| 22  | b     | 6024 | CLA  | C3C-C2C | 4.80  | 1.47        | 1.36     |
| 22  | C     | 1029 | CLA  | C3D-C4D | -4.80 | 1.33        | 1.44     |
| 22  | b     | 6022 | CLA  | C3C-C2C | 4.79  | 1.47        | 1.36     |
| 22  | C     | 1033 | CLA  | C3C-C2C | 4.79  | 1.47        | 1.36     |
| 22  | C     | 1030 | CLA  | C3D-C4D | -4.79 | 1.33        | 1.44     |
| 22  | c     | 6036 | CLA  | C3C-C2C | 4.79  | 1.47        | 1.36     |
| 22  | C     | 1028 | CLA  | C3C-C2C | 4.79  | 1.47        | 1.36     |
| 22  | B     | 1021 | CLA  | C3D-C4D | -4.79 | 1.33        | 1.44     |
| 22  | c     | 6033 | CLA  | C3C-C2C | 4.78  | 1.47        | 1.36     |
| 22  | B     | 1019 | CLA  | C3C-C2C | 4.78  | 1.47        | 1.36     |
| 23  | D     | 1039 | PHO  | C3D-C2D | 4.78  | 1.47        | 1.39     |
| 23  | a     | 6038 | PHO  | C3D-C2D | 4.78  | 1.47        | 1.39     |
| 22  | c     | 6037 | CLA  | C3C-C2C | 4.78  | 1.47        | 1.36     |
| 22  | B     | 1009 | CLA  | C3C-C2C | 4.78  | 1.47        | 1.36     |
| 22  | b     | 6009 | CLA  | C3C-C2C | 4.77  | 1.47        | 1.36     |
| 22  | b     | 6019 | CLA  | C3C-C2C | 4.76  | 1.47        | 1.36     |
| 22  | B     | 1023 | CLA  | C3D-C4D | -4.76 | 1.33        | 1.44     |
| 22  | b     | 6023 | CLA  | C3D-C4D | -4.75 | 1.33        | 1.44     |
| 22  | B     | 1010 | CLA  | C3C-C2C | 4.74  | 1.47        | 1.36     |
| 22  | C     | 1030 | CLA  | C3C-C2C | 4.73  | 1.47        | 1.36     |
| 22  | c     | 6030 | CLA  | C3C-C2C | 4.73  | 1.47        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | b     | 6011 | CLA  | C3C-C2C | 4.73  | 1.47        | 1.36     |
| 22  | b     | 6021 | CLA  | C3C-C2C | 4.72  | 1.47        | 1.36     |
| 22  | B     | 1009 | CLA  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 22  | B     | 1011 | CLA  | C3C-C2C | 4.72  | 1.46        | 1.36     |
| 22  | B     | 1021 | CLA  | C3C-C2C | 4.71  | 1.46        | 1.36     |
| 22  | b     | 6010 | CLA  | C3C-C2C | 4.71  | 1.46        | 1.36     |
| 22  | c     | 6036 | CLA  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 22  | b     | 6014 | CLA  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 22  | h     | 6017 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 22  | c     | 6027 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 22  | b     | 6012 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 22  | b     | 6009 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 22  | C     | 1036 | CLA  | C3D-C4D | -4.69 | 1.33        | 1.44     |
| 22  | a     | 6007 | CLA  | C3D-C4D | -4.69 | 1.33        | 1.44     |
| 22  | A     | 1006 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | C     | 1029 | CLA  | C3C-C2C | 4.68  | 1.46        | 1.36     |
| 22  | b     | 6022 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | H     | 1017 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | B     | 1012 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | C     | 1027 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | c     | 6032 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | D     | 1005 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | d     | 6005 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 22  | a     | 6006 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | d     | 6004 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | B     | 1022 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | C     | 1037 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | D     | 1004 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | b     | 6018 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | B     | 1014 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | c     | 6029 | CLA  | C3C-C2C | 4.67  | 1.46        | 1.36     |
| 22  | C     | 1033 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | A     | 1007 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | C     | 1026 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | B     | 1015 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | b     | 6023 | CLA  | C3C-C2C | 4.67  | 1.46        | 1.36     |
| 22  | b     | 6015 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | C     | 1032 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | c     | 6025 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 22  | C     | 1025 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | C     | 1035 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | b     | 6020 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1019 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | B     | 1018 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | K     | 1034 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | B     | 1023 | CLA  | C3C-C2C | 4.66  | 1.46        | 1.36     |
| 22  | B     | 1016 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | b     | 6024 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | b     | 6016 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | c     | 6037 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | k     | 6034 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 22  | b     | 6019 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 22  | c     | 6026 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 22  | C     | 1028 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 22  | C     | 1031 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 22  | B     | 1024 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 22  | c     | 6028 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 22  | B     | 1020 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 22  | c     | 6035 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 22  | c     | 6033 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 22  | D     | 1008 | CLA  | C3C-C2C | 4.63  | 1.46        | 1.36     |
| 22  | B     | 1013 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 23  | d     | 6039 | PHO  | C3D-CAD | -4.63 | 1.38        | 1.47     |
| 22  | b     | 6013 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 22  | c     | 6031 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 22  | d     | 6008 | CLA  | C3C-C2C | 4.63  | 1.46        | 1.36     |
| 22  | A     | 1003 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 23  | D     | 1039 | PHO  | C3D-CAD | -4.62 | 1.38        | 1.47     |
| 22  | a     | 6003 | CLA  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 23  | A     | 1038 | PHO  | C3D-CAD | -4.59 | 1.39        | 1.47     |
| 23  | a     | 6038 | PHO  | C3D-CAD | -4.59 | 1.39        | 1.47     |
| 22  | d     | 6005 | CLA  | CHC-C1C | 4.56  | 1.47        | 1.38     |
| 22  | c     | 6033 | CLA  | CHC-C1C | 4.55  | 1.47        | 1.38     |
| 22  | D     | 1005 | CLA  | CHC-C1C | 4.54  | 1.47        | 1.38     |
| 22  | C     | 1035 | CLA  | CHC-C1C | 4.54  | 1.47        | 1.38     |
| 22  | c     | 6035 | CLA  | CHC-C1C | 4.53  | 1.47        | 1.38     |
| 22  | b     | 6024 | CLA  | CHC-C1C | 4.53  | 1.47        | 1.38     |
| 22  | B     | 1016 | CLA  | CHC-C1C | 4.52  | 1.47        | 1.38     |
| 22  | A     | 1007 | CLA  | CHC-C1C | 4.52  | 1.47        | 1.38     |
| 22  | a     | 6007 | CLA  | CHC-C1C | 4.51  | 1.47        | 1.38     |
| 22  | C     | 1033 | CLA  | CHC-C1C | 4.51  | 1.47        | 1.38     |
| 22  | c     | 6026 | CLA  | CHC-C1C | 4.51  | 1.47        | 1.38     |
| 22  | b     | 6014 | CLA  | CHC-C1C | 4.51  | 1.47        | 1.38     |
| 22  | k     | 6034 | CLA  | CHC-C1C | 4.51  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | b     | 6013 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | B     | 1024 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | D     | 1004 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | a     | 6006 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | B     | 1020 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | K     | 1034 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | a     | 6003 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | C     | 1028 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | B     | 1014 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 22  | C     | 1025 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | C     | 1026 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | C     | 1031 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | B     | 1013 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | c     | 6028 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | c     | 6031 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | B     | 1019 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | A     | 1003 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | B     | 1018 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | b     | 6012 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | c     | 6025 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 22  | H     | 1017 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | b     | 6016 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | b     | 6019 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | b     | 6020 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | B     | 1012 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | b     | 6018 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | C     | 1032 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | c     | 6032 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | c     | 6036 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | C     | 1027 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 22  | B     | 1022 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 22  | A     | 1006 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 22  | b     | 6022 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 22  | d     | 6004 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 22  | B     | 1015 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 22  | C     | 1037 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 22  | c     | 6030 | CLA  | CHC-C1C | 4.46 | 1.47        | 1.38     |
| 22  | c     | 6027 | CLA  | CHC-C1C | 4.45 | 1.47        | 1.38     |
| 22  | C     | 1036 | CLA  | CHC-C1C | 4.45 | 1.47        | 1.38     |
| 22  | B     | 1018 | CLA  | CHD-C1D | 4.45 | 1.47        | 1.38     |
| 22  | C     | 1030 | CLA  | CHC-C1C | 4.45 | 1.47        | 1.38     |
| 22  | b     | 6018 | CLA  | CHD-C1D | 4.45 | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | h     | 6017 | CLA  | CHC-C1C | 4.44 | 1.47        | 1.38     |
| 22  | a     | 6007 | CLA  | CHD-C1D | 4.44 | 1.47        | 1.38     |
| 22  | c     | 6037 | CLA  | CHC-C1C | 4.44 | 1.47        | 1.38     |
| 22  | b     | 6015 | CLA  | CHC-C1C | 4.44 | 1.47        | 1.38     |
| 22  | c     | 6025 | CLA  | CHD-C1D | 4.43 | 1.47        | 1.38     |
| 22  | b     | 6016 | CLA  | CHD-C1D | 4.43 | 1.47        | 1.38     |
| 22  | b     | 6020 | CLA  | CHD-C1D | 4.43 | 1.47        | 1.38     |
| 22  | A     | 1007 | CLA  | CHD-C1D | 4.42 | 1.47        | 1.38     |
| 22  | d     | 6004 | CLA  | CHD-C1D | 4.41 | 1.47        | 1.38     |
| 31  | f     | 6040 | HEM  | FE-ND   | 4.41 | 2.08        | 1.94     |
| 22  | d     | 6005 | CLA  | CHD-C1D | 4.41 | 1.47        | 1.38     |
| 31  | v     | 6041 | HEM  | FE-ND   | 4.41 | 2.08        | 1.94     |
| 22  | D     | 1004 | CLA  | CHD-C1D | 4.41 | 1.47        | 1.38     |
| 31  | V     | 1041 | HEM  | FE-ND   | 4.41 | 2.08        | 1.94     |
| 22  | b     | 6021 | CLA  | CHC-C1C | 4.41 | 1.47        | 1.38     |
| 31  | F     | 1040 | HEM  | FE-ND   | 4.41 | 2.08        | 1.94     |
| 22  | C     | 1025 | CLA  | CHD-C1D | 4.41 | 1.47        | 1.38     |
| 22  | b     | 6013 | CLA  | CHD-C1D | 4.41 | 1.47        | 1.38     |
| 22  | h     | 6017 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | B     | 1014 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | a     | 6003 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | B     | 1021 | CLA  | CHC-C1C | 4.40 | 1.47        | 1.38     |
| 22  | B     | 1020 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | D     | 1005 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | B     | 1012 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | C     | 1032 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | c     | 6031 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | A     | 1003 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | c     | 6036 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | k     | 6034 | CLA  | CHD-C1D | 4.40 | 1.47        | 1.38     |
| 22  | c     | 6027 | CLA  | CHD-C1D | 4.39 | 1.47        | 1.38     |
| 22  | C     | 1036 | CLA  | CHD-C1D | 4.39 | 1.47        | 1.38     |
| 22  | K     | 1034 | CLA  | CHD-C1D | 4.39 | 1.47        | 1.38     |
| 22  | b     | 6023 | CLA  | CHC-C1C | 4.39 | 1.47        | 1.38     |
| 22  | B     | 1024 | CLA  | CHD-C1D | 4.39 | 1.47        | 1.38     |
| 22  | C     | 1031 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | c     | 6032 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | b     | 6019 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | B     | 1013 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | B     | 1015 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | C     | 1033 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | b     | 6015 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | C     | 1028 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | H     | 1017 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | B     | 1016 | CLA  | CHD-C1D | 4.38 | 1.47        | 1.38     |
| 22  | A     | 1006 | CLA  | CHD-C1D | 4.37 | 1.47        | 1.38     |
| 22  | b     | 6012 | CLA  | CHD-C1D | 4.37 | 1.47        | 1.38     |
| 22  | C     | 1027 | CLA  | CHD-C1D | 4.37 | 1.47        | 1.38     |
| 22  | C     | 1029 | CLA  | CHC-C1C | 4.37 | 1.47        | 1.38     |
| 22  | C     | 1037 | CLA  | CHD-C1D | 4.37 | 1.47        | 1.38     |
| 22  | C     | 1026 | CLA  | CHD-C1D | 4.37 | 1.46        | 1.38     |
| 22  | b     | 6014 | CLA  | CHD-C1D | 4.37 | 1.46        | 1.38     |
| 22  | B     | 1022 | CLA  | CHD-C1D | 4.37 | 1.46        | 1.38     |
| 22  | B     | 1023 | CLA  | CHC-C1C | 4.37 | 1.47        | 1.38     |
| 22  | c     | 6026 | CLA  | CHD-C1D | 4.36 | 1.46        | 1.38     |
| 22  | B     | 1010 | CLA  | CHC-C1C | 4.36 | 1.47        | 1.38     |
| 22  | C     | 1035 | CLA  | CHD-C1D | 4.36 | 1.46        | 1.38     |
| 22  | c     | 6029 | CLA  | CHC-C1C | 4.36 | 1.47        | 1.38     |
| 22  | b     | 6024 | CLA  | CHD-C1D | 4.36 | 1.46        | 1.38     |
| 22  | a     | 6006 | CLA  | CHD-C1D | 4.36 | 1.46        | 1.38     |
| 22  | B     | 1019 | CLA  | CHD-C1D | 4.36 | 1.46        | 1.38     |
| 22  | c     | 6028 | CLA  | CHD-C1D | 4.36 | 1.46        | 1.38     |
| 22  | c     | 6035 | CLA  | CHD-C1D | 4.36 | 1.46        | 1.38     |
| 22  | c     | 6033 | CLA  | CHD-C1D | 4.35 | 1.46        | 1.38     |
| 22  | b     | 6022 | CLA  | CHD-C1D | 4.35 | 1.46        | 1.38     |
| 22  | c     | 6037 | CLA  | CHD-C1D | 4.35 | 1.46        | 1.38     |
| 22  | b     | 6010 | CLA  | CHC-C1C | 4.34 | 1.47        | 1.38     |
| 22  | d     | 6008 | CLA  | CHC-C1C | 4.34 | 1.47        | 1.38     |
| 22  | B     | 1011 | CLA  | CHC-C1C | 4.33 | 1.47        | 1.38     |
| 22  | D     | 1008 | CLA  | CHC-C1C | 4.33 | 1.47        | 1.38     |
| 22  | d     | 6005 | CLA  | O2A-CGA | 4.33 | 1.46        | 1.33     |
| 29  | c     | 6057 | DGD  | O1G-C1A | 4.32 | 1.45        | 1.33     |
| 29  | c     | 6055 | DGD  | O1G-C1A | 4.32 | 1.45        | 1.33     |
| 22  | d     | 6008 | CLA  | CHD-C1D | 4.32 | 1.46        | 1.38     |
| 22  | D     | 1005 | CLA  | O2A-CGA | 4.32 | 1.45        | 1.33     |
| 29  | b     | 6058 | DGD  | O1G-C1A | 4.31 | 1.45        | 1.33     |
| 22  | c     | 6037 | CLA  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 22  | b     | 6015 | CLA  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 22  | B     | 1010 | CLA  | CHD-C1D | 4.31 | 1.46        | 1.38     |
| 22  | b     | 6016 | CLA  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 22  | c     | 6033 | CLA  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 29  | B     | 1058 | DGD  | O1G-C1A | 4.31 | 1.45        | 1.33     |
| 22  | c     | 6031 | CLA  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 22  | b     | 6011 | CLA  | CHC-C1C | 4.30 | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 28  | b     | 6060 | MGE  | O1G-C1A | 4.30  | 1.45        | 1.33     |
| 28  | d     | 6062 | MGE  | O1G-C1A | 4.30  | 1.45        | 1.33     |
| 25  | z     | 6053 | BCR  | C17-C18 | -4.30 | 1.25        | 1.35     |
| 22  | C     | 1032 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 22  | C     | 1037 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 25  | k     | 6052 | BCR  | C17-C18 | -4.30 | 1.25        | 1.35     |
| 22  | b     | 6024 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 22  | b     | 6012 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 22  | B     | 1022 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 22  | b     | 6022 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 26  | A     | 1063 | LHG  | O8-C23  | 4.30  | 1.45        | 1.33     |
| 22  | B     | 1009 | CLA  | CHC-C1C | 4.30  | 1.47        | 1.38     |
| 22  | d     | 6004 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 22  | D     | 1004 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 29  | C     | 1055 | DGD  | O1G-C1A | 4.30  | 1.45        | 1.33     |
| 28  | D     | 1062 | MGE  | O1G-C1A | 4.30  | 1.45        | 1.33     |
| 22  | B     | 1013 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 22  | B     | 1021 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 25  | d     | 6050 | BCR  | C21-C22 | -4.29 | 1.25        | 1.35     |
| 22  | C     | 1025 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | B     | 1016 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | C     | 1033 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | b     | 6023 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 22  | k     | 6034 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | B     | 1020 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | C     | 1030 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | b     | 6013 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 25  | T     | 6048 | BCR  | C21-C22 | -4.29 | 1.25        | 1.35     |
| 25  | D     | 1050 | BCR  | C21-C22 | -4.29 | 1.25        | 1.35     |
| 26  | a     | 6063 | LHG  | O8-C23  | 4.29  | 1.45        | 1.33     |
| 22  | c     | 6032 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 28  | D     | 1059 | MGE  | O1G-C1A | 4.29  | 1.45        | 1.33     |
| 29  | C     | 1057 | DGD  | O1G-C1A | 4.29  | 1.45        | 1.33     |
| 25  | B     | 1048 | BCR  | C17-C18 | -4.29 | 1.25        | 1.35     |
| 22  | B     | 1012 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | b     | 6010 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 22  | b     | 6014 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 22  | b     | 6019 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 28  | L     | 1061 | MGE  | O1G-C1A | 4.29  | 1.45        | 1.33     |
| 22  | c     | 6029 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 22  | B     | 1024 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 28  | B     | 1060 | MGE  | O1G-C1A | 4.29  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | C     | 1031 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | B     | 1009 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 22  | a     | 6006 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 28  | d     | 6059 | MGE  | O1G-C1A | 4.28  | 1.45        | 1.33     |
| 25  | Z     | 1053 | BCR  | C21-C22 | -4.28 | 1.25        | 1.35     |
| 22  | b     | 6009 | CLA  | CHC-C1C | 4.28  | 1.47        | 1.38     |
| 22  | C     | 1036 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | B     | 1015 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | B     | 1019 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | C     | 1035 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | B     | 1018 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | C     | 1026 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 29  | C     | 1056 | DGD  | O1G-C1A | 4.28  | 1.45        | 1.33     |
| 29  | c     | 6056 | DGD  | O1G-C1A | 4.28  | 1.45        | 1.33     |
| 22  | c     | 6030 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | K     | 1034 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | b     | 6018 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 25  | b     | 6047 | BCR  | C21-C22 | -4.28 | 1.25        | 1.35     |
| 22  | a     | 6007 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | B     | 1014 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | b     | 6009 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 22  | c     | 6035 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 22  | A     | 1006 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 22  | c     | 6025 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 22  | c     | 6036 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 22  | C     | 1028 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 25  | z     | 6053 | BCR  | C21-C22 | -4.27 | 1.25        | 1.35     |
| 22  | A     | 1007 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 22  | H     | 1017 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 22  | D     | 1008 | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 22  | C     | 1027 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 25  | Z     | 1053 | BCR  | C17-C18 | -4.27 | 1.25        | 1.35     |
| 25  | D     | 1050 | BCR  | C17-C18 | -4.27 | 1.25        | 1.35     |
| 22  | b     | 6020 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 25  | H     | 1049 | BCR  | C21-C22 | -4.27 | 1.25        | 1.35     |
| 28  | l     | 6061 | MGE  | O1G-C1A | 4.26  | 1.45        | 1.33     |
| 22  | c     | 6029 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 22  | c     | 6028 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 22  | C     | 1029 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 22  | b     | 6021 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 22  | B     | 1023 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 22  | c     | 6026 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1009 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 22  | B     | 1010 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 25  | C     | 1054 | BCR  | C17-C18 | -4.26 | 1.25        | 1.35     |
| 22  | A     | 1003 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 25  | B     | 1045 | BCR  | C17-C18 | -4.26 | 1.26        | 1.35     |
| 22  | B     | 1011 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 22  | D     | 1008 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 22  | c     | 6027 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 22  | h     | 6017 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 25  | C     | 1052 | BCR  | C17-C18 | -4.25 | 1.26        | 1.35     |
| 25  | B     | 1048 | BCR  | C21-C22 | -4.25 | 1.26        | 1.35     |
| 25  | B     | 1047 | BCR  | C21-C22 | -4.25 | 1.26        | 1.35     |
| 25  | K     | 1051 | BCR  | C21-C22 | -4.25 | 1.26        | 1.35     |
| 22  | d     | 6008 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 25  | b     | 6045 | BCR  | C17-C18 | -4.25 | 1.26        | 1.35     |
| 25  | B     | 1047 | BCR  | C17-C18 | -4.25 | 1.26        | 1.35     |
| 25  | T     | 6048 | BCR  | C17-C18 | -4.25 | 1.26        | 1.35     |
| 22  | a     | 6003 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 25  | C     | 1054 | BCR  | C21-C22 | -4.25 | 1.26        | 1.35     |
| 22  | B     | 1021 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 22  | C     | 1029 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 25  | K     | 1051 | BCR  | C17-C18 | -4.25 | 1.26        | 1.35     |
| 22  | B     | 1023 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 25  | k     | 6051 | BCR  | C21-C22 | -4.25 | 1.26        | 1.35     |
| 25  | H     | 1049 | BCR  | C17-C18 | -4.24 | 1.26        | 1.35     |
| 22  | b     | 6011 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 25  | k     | 6051 | BCR  | C17-C18 | -4.24 | 1.26        | 1.35     |
| 25  | d     | 6050 | BCR  | C17-C18 | -4.24 | 1.26        | 1.35     |
| 25  | k     | 6052 | BCR  | C21-C22 | -4.24 | 1.26        | 1.35     |
| 22  | b     | 6010 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 22  | b     | 6009 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 25  | c     | 6054 | BCR  | C21-C22 | -4.24 | 1.26        | 1.35     |
| 22  | b     | 6011 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 25  | B     | 1045 | BCR  | C21-C22 | -4.24 | 1.26        | 1.35     |
| 25  | C     | 1052 | BCR  | C21-C22 | -4.24 | 1.26        | 1.35     |
| 25  | c     | 6054 | BCR  | C17-C18 | -4.24 | 1.26        | 1.35     |
| 25  | h     | 6049 | BCR  | C21-C22 | -4.24 | 1.26        | 1.35     |
| 22  | b     | 6023 | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 25  | b     | 6045 | BCR  | C21-C22 | -4.23 | 1.26        | 1.35     |
| 25  | b     | 6047 | BCR  | C17-C18 | -4.22 | 1.26        | 1.35     |
| 22  | c     | 6030 | CLA  | CHD-C1D | 4.22  | 1.46        | 1.38     |
| 22  | B     | 1011 | CLA  | O2A-CGA | 4.22  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | h     | 6049 | BCR  | C17-C18 | -4.22 | 1.26        | 1.35     |
| 22  | b     | 6021 | CLA  | O2A-CGA | 4.22  | 1.45        | 1.33     |
| 22  | C     | 1030 | CLA  | CHD-C1D | 4.21  | 1.46        | 1.38     |
| 25  | T     | 6046 | BCR  | C17-C18 | -4.14 | 1.26        | 1.35     |
| 25  | A     | 1044 | BCR  | C17-C18 | -4.13 | 1.26        | 1.35     |
| 26  | A     | 1063 | LHG  | O7-C7   | 4.13  | 1.45        | 1.34     |
| 25  | t     | 1046 | BCR  | C17-C18 | -4.12 | 1.26        | 1.35     |
| 26  | a     | 6063 | LHG  | O7-C7   | 4.12  | 1.45        | 1.34     |
| 25  | A     | 1044 | BCR  | C21-C22 | -4.12 | 1.26        | 1.35     |
| 29  | c     | 6055 | DGD  | O2G-C1B | 4.12  | 1.45        | 1.34     |
| 28  | l     | 6061 | MGE  | O2G-C1B | 4.12  | 1.45        | 1.34     |
| 22  | b     | 6015 | CLA  | CHD-C4C | 4.11  | 1.48        | 1.39     |
| 22  | c     | 6035 | CLA  | CHD-C4C | 4.11  | 1.48        | 1.39     |
| 25  | a     | 6044 | BCR  | C21-C22 | -4.11 | 1.26        | 1.35     |
| 28  | d     | 6062 | MGE  | O2G-C1B | 4.11  | 1.45        | 1.34     |
| 22  | C     | 1027 | CLA  | CHD-C4C | 4.11  | 1.48        | 1.39     |
| 22  | b     | 6020 | CLA  | CHD-C4C | 4.11  | 1.48        | 1.39     |
| 28  | d     | 6059 | MGE  | O2G-C1B | 4.11  | 1.45        | 1.34     |
| 22  | b     | 6022 | CLA  | CHD-C4C | 4.11  | 1.48        | 1.39     |
| 28  | D     | 1059 | MGE  | O2G-C1B | 4.11  | 1.45        | 1.34     |
| 29  | C     | 1055 | DGD  | O2G-C1B | 4.11  | 1.45        | 1.34     |
| 29  | B     | 1058 | DGD  | O2G-C1B | 4.11  | 1.45        | 1.34     |
| 28  | b     | 6060 | MGE  | O2G-C1B | 4.10  | 1.45        | 1.34     |
| 22  | B     | 1015 | CLA  | CHD-C4C | 4.10  | 1.48        | 1.39     |
| 22  | c     | 6027 | CLA  | CHD-C4C | 4.10  | 1.48        | 1.39     |
| 28  | D     | 1062 | MGE  | O2G-C1B | 4.10  | 1.45        | 1.34     |
| 22  | D     | 1004 | CLA  | CHD-C4C | 4.10  | 1.48        | 1.39     |
| 29  | b     | 6058 | DGD  | O2G-C1B | 4.10  | 1.45        | 1.34     |
| 22  | B     | 1020 | CLA  | CHD-C4C | 4.10  | 1.48        | 1.39     |
| 28  | L     | 1061 | MGE  | O2G-C1B | 4.10  | 1.45        | 1.34     |
| 22  | B     | 1014 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 28  | B     | 1060 | MGE  | O2G-C1B | 4.09  | 1.45        | 1.34     |
| 22  | d     | 6004 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 22  | B     | 1013 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 25  | a     | 6044 | BCR  | C17-C18 | -4.09 | 1.26        | 1.35     |
| 22  | c     | 6033 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 22  | K     | 1034 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 22  | c     | 6025 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 29  | c     | 6056 | DGD  | O2G-C1B | 4.09  | 1.45        | 1.34     |
| 22  | C     | 1025 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 29  | C     | 1057 | DGD  | O2G-C1B | 4.09  | 1.45        | 1.34     |
| 22  | b     | 6016 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | c     | 6028 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 22  | k     | 6034 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 25  | T     | 6046 | BCR  | C21-C22 | -4.09 | 1.26        | 1.35     |
| 22  | B     | 1016 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | H     | 1017 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | B     | 1022 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | h     | 6017 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | C     | 1033 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | c     | 6036 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | C     | 1032 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | a     | 6003 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | b     | 6019 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | c     | 6032 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | C     | 1031 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | c     | 6026 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | C     | 1037 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 22  | c     | 6037 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 29  | c     | 6057 | DGD  | O2G-C1B | 4.08  | 1.45        | 1.34     |
| 22  | b     | 6014 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 22  | C     | 1035 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 29  | C     | 1056 | DGD  | O2G-C1B | 4.07  | 1.45        | 1.34     |
| 31  | v     | 6041 | HEM  | FE-NB   | 4.07  | 2.07        | 1.94     |
| 22  | C     | 1028 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 22  | A     | 1003 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 22  | C     | 1036 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 31  | f     | 6040 | HEM  | FE-NB   | 4.06  | 2.07        | 1.94     |
| 22  | C     | 1026 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 22  | B     | 1024 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 25  | t     | 1046 | BCR  | C21-C22 | -4.06 | 1.26        | 1.35     |
| 22  | B     | 1019 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 31  | V     | 1041 | HEM  | FE-NB   | 4.06  | 2.07        | 1.94     |
| 22  | b     | 6013 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 22  | B     | 1012 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 22  | A     | 1006 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 31  | F     | 1040 | HEM  | FE-NB   | 4.05  | 2.07        | 1.94     |
| 22  | a     | 6006 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 22  | b     | 6024 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 22  | c     | 6031 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 22  | b     | 6018 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 22  | D     | 1005 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 22  | d     | 6005 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 22  | A     | 1007 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | a     | 6007 | CLA  | CHD-C4C | 4.03 | 1.48        | 1.39     |
| 22  | b     | 6012 | CLA  | CHD-C4C | 4.03 | 1.48        | 1.39     |
| 22  | B     | 1018 | CLA  | CHD-C4C | 4.03 | 1.48        | 1.39     |
| 22  | b     | 6010 | CLA  | CHD-C4C | 4.02 | 1.48        | 1.39     |
| 22  | d     | 6008 | CLA  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 22  | B     | 1021 | CLA  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 22  | D     | 1008 | CLA  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 22  | b     | 6021 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 22  | C     | 1029 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 22  | B     | 1010 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 22  | b     | 6023 | CLA  | CHD-C4C | 3.98 | 1.48        | 1.39     |
| 22  | B     | 1023 | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 22  | C     | 1030 | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 22  | B     | 1009 | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 22  | b     | 6009 | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 22  | b     | 6011 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 22  | B     | 1011 | CLA  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 22  | c     | 6029 | CLA  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 22  | c     | 6030 | CLA  | CHD-C4C | 3.93 | 1.48        | 1.39     |
| 22  | c     | 6037 | CLA  | OBD-CAD | 3.83 | 1.29        | 1.22     |
| 22  | b     | 6014 | CLA  | OBD-CAD | 3.83 | 1.29        | 1.22     |
| 22  | c     | 6035 | CLA  | OBD-CAD | 3.81 | 1.29        | 1.22     |
| 22  | B     | 1014 | CLA  | OBD-CAD | 3.81 | 1.29        | 1.22     |
| 22  | h     | 6017 | CLA  | OBD-CAD | 3.81 | 1.29        | 1.22     |
| 22  | c     | 6032 | CLA  | OBD-CAD | 3.79 | 1.29        | 1.22     |
| 22  | C     | 1025 | CLA  | OBD-CAD | 3.79 | 1.29        | 1.22     |
| 22  | C     | 1037 | CLA  | OBD-CAD | 3.79 | 1.29        | 1.22     |
| 22  | D     | 1004 | CLA  | OBD-CAD | 3.79 | 1.29        | 1.22     |
| 22  | C     | 1032 | CLA  | OBD-CAD | 3.78 | 1.29        | 1.22     |
| 22  | C     | 1035 | CLA  | OBD-CAD | 3.78 | 1.29        | 1.22     |
| 22  | c     | 6025 | CLA  | OBD-CAD | 3.78 | 1.29        | 1.22     |
| 22  | b     | 6015 | CLA  | OBD-CAD | 3.78 | 1.29        | 1.22     |
| 22  | b     | 6019 | CLA  | OBD-CAD | 3.78 | 1.29        | 1.22     |
| 22  | b     | 6018 | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 22  | b     | 6021 | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 22  | B     | 1024 | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 22  | d     | 6004 | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 22  | c     | 6033 | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 22  | C     | 1036 | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 22  | k     | 6034 | CLA  | OBD-CAD | 3.76 | 1.29        | 1.22     |
| 22  | B     | 1015 | CLA  | OBD-CAD | 3.76 | 1.29        | 1.22     |
| 22  | B     | 1019 | CLA  | OBD-CAD | 3.76 | 1.29        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | B     | 1018 | CLA  | OBD-CAD | 3.76 | 1.29        | 1.22     |
| 22  | H     | 1017 | CLA  | OBD-CAD | 3.76 | 1.29        | 1.22     |
| 22  | C     | 1028 | CLA  | OBD-CAD | 3.76 | 1.29        | 1.22     |
| 22  | B     | 1020 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | C     | 1033 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | c     | 6031 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | B     | 1021 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | B     | 1022 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | C     | 1031 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | b     | 6024 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | c     | 6027 | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 22  | B     | 1013 | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 22  | B     | 1012 | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 22  | a     | 6003 | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 22  | D     | 1005 | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 22  | c     | 6028 | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 22  | A     | 1006 | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 22  | b     | 6022 | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 22  | C     | 1027 | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 22  | b     | 6016 | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 22  | B     | 1016 | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 22  | d     | 6005 | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 22  | b     | 6012 | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 22  | b     | 6020 | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 22  | c     | 6036 | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 22  | a     | 6007 | CLA  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 22  | A     | 1007 | CLA  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 22  | K     | 1034 | CLA  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 22  | A     | 1003 | CLA  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 22  | c     | 6026 | CLA  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 22  | b     | 6013 | CLA  | OBD-CAD | 3.71 | 1.28        | 1.22     |
| 22  | a     | 6006 | CLA  | OBD-CAD | 3.70 | 1.28        | 1.22     |
| 22  | C     | 1026 | CLA  | OBD-CAD | 3.70 | 1.28        | 1.22     |
| 22  | b     | 6011 | CLA  | OBD-CAD | 3.68 | 1.28        | 1.22     |
| 22  | B     | 1011 | CLA  | OBD-CAD | 3.65 | 1.28        | 1.22     |
| 22  | b     | 6009 | CLA  | OBD-CAD | 3.62 | 1.28        | 1.22     |
| 22  | B     | 1023 | CLA  | OBD-CAD | 3.61 | 1.28        | 1.22     |
| 22  | b     | 6023 | CLA  | OBD-CAD | 3.61 | 1.28        | 1.22     |
| 22  | c     | 6029 | CLA  | OBD-CAD | 3.61 | 1.28        | 1.22     |
| 22  | B     | 1009 | CLA  | OBD-CAD | 3.60 | 1.28        | 1.22     |
| 22  | C     | 1030 | CLA  | OBD-CAD | 3.59 | 1.28        | 1.22     |
| 22  | D     | 1008 | CLA  | OBD-CAD | 3.59 | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | b     | 6010 | CLA  | OBD-CAD | 3.58 | 1.28        | 1.22     |
| 22  | d     | 6008 | CLA  | OBD-CAD | 3.58 | 1.28        | 1.22     |
| 22  | C     | 1029 | CLA  | OBD-CAD | 3.58 | 1.28        | 1.22     |
| 22  | a     | 6007 | CLA  | CHC-C4B | 3.57 | 1.47        | 1.39     |
| 22  | c     | 6037 | CLA  | CHC-C4B | 3.56 | 1.47        | 1.39     |
| 22  | b     | 6015 | CLA  | CHC-C4B | 3.56 | 1.47        | 1.39     |
| 22  | c     | 6030 | CLA  | OBD-CAD | 3.54 | 1.28        | 1.22     |
| 22  | b     | 6020 | CLA  | CHC-C4B | 3.54 | 1.47        | 1.39     |
| 22  | B     | 1015 | CLA  | CHC-C4B | 3.54 | 1.47        | 1.39     |
| 22  | H     | 1017 | CLA  | CHC-C4B | 3.54 | 1.47        | 1.39     |
| 22  | B     | 1010 | CLA  | OBD-CAD | 3.54 | 1.28        | 1.22     |
| 22  | C     | 1037 | CLA  | CHC-C4B | 3.54 | 1.47        | 1.39     |
| 22  | b     | 6018 | CLA  | CHC-C4B | 3.53 | 1.47        | 1.39     |
| 22  | c     | 6036 | CLA  | CHC-C4B | 3.53 | 1.47        | 1.39     |
| 22  | A     | 1007 | CLA  | CHC-C4B | 3.53 | 1.47        | 1.39     |
| 22  | c     | 6027 | CLA  | CHC-C4B | 3.53 | 1.47        | 1.39     |
| 22  | a     | 6003 | CLA  | CHC-C4B | 3.53 | 1.47        | 1.39     |
| 22  | b     | 6012 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | b     | 6016 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | k     | 6034 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | B     | 1013 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | B     | 1016 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | B     | 1012 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | B     | 1020 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | A     | 1003 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | B     | 1018 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | b     | 6013 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | h     | 6017 | CLA  | CHC-C4B | 3.52 | 1.47        | 1.39     |
| 22  | B     | 1022 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | C     | 1035 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | a     | 6006 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | c     | 6033 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | C     | 1027 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | c     | 6026 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | C     | 1026 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | b     | 6019 | CLA  | CHC-C4B | 3.51 | 1.47        | 1.39     |
| 22  | c     | 6031 | CLA  | CHC-C4B | 3.50 | 1.47        | 1.39     |
| 22  | B     | 1019 | CLA  | CHC-C4B | 3.50 | 1.47        | 1.39     |
| 22  | C     | 1036 | CLA  | CHC-C4B | 3.50 | 1.47        | 1.39     |
| 22  | A     | 1006 | CLA  | CHC-C4B | 3.50 | 1.47        | 1.39     |
| 22  | C     | 1031 | CLA  | CHC-C4B | 3.50 | 1.47        | 1.39     |
| 22  | b     | 6022 | CLA  | CHC-C4B | 3.50 | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | C     | 1025 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | c     | 6025 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | C     | 1032 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | K     | 1034 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | D     | 1004 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | C     | 1033 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | B     | 1014 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | c     | 6035 | CLA  | CHC-C4B | 3.49 | 1.47        | 1.39     |
| 22  | c     | 6032 | CLA  | CHC-C4B | 3.48 | 1.47        | 1.39     |
| 22  | b     | 6023 | CLA  | CHC-C4B | 3.47 | 1.47        | 1.39     |
| 22  | D     | 1005 | CLA  | CHC-C4B | 3.47 | 1.47        | 1.39     |
| 22  | c     | 6028 | CLA  | CHC-C4B | 3.47 | 1.47        | 1.39     |
| 22  | B     | 1024 | CLA  | CHC-C4B | 3.47 | 1.47        | 1.39     |
| 22  | C     | 1028 | CLA  | CHC-C4B | 3.47 | 1.47        | 1.39     |
| 22  | b     | 6014 | CLA  | CHC-C4B | 3.47 | 1.47        | 1.39     |
| 22  | d     | 6005 | CLA  | CHC-C4B | 3.46 | 1.47        | 1.39     |
| 22  | b     | 6024 | CLA  | CHC-C4B | 3.46 | 1.47        | 1.39     |
| 22  | d     | 6004 | CLA  | CHC-C4B | 3.45 | 1.47        | 1.39     |
| 22  | B     | 1023 | CLA  | CHC-C4B | 3.45 | 1.47        | 1.39     |
| 22  | b     | 6011 | CLA  | CHC-C4B | 3.42 | 1.47        | 1.39     |
| 22  | b     | 6009 | CLA  | CHC-C4B | 3.41 | 1.47        | 1.39     |
| 22  | B     | 1009 | CLA  | CHC-C4B | 3.41 | 1.47        | 1.39     |
| 22  | B     | 1021 | CLA  | CHC-C4B | 3.40 | 1.47        | 1.39     |
| 22  | b     | 6010 | CLA  | CHC-C4B | 3.40 | 1.47        | 1.39     |
| 22  | B     | 1011 | CLA  | CHC-C4B | 3.39 | 1.47        | 1.39     |
| 23  | d     | 6039 | PHO  | CBB-CAB | 3.38 | 1.50        | 1.29     |
| 22  | C     | 1030 | CLA  | CHC-C4B | 3.38 | 1.47        | 1.39     |
| 23  | D     | 1039 | PHO  | CBB-CAB | 3.38 | 1.50        | 1.29     |
| 22  | d     | 6008 | CLA  | CHC-C4B | 3.38 | 1.47        | 1.39     |
| 22  | B     | 1010 | CLA  | CHC-C4B | 3.37 | 1.47        | 1.39     |
| 22  | c     | 6030 | CLA  | CHC-C4B | 3.37 | 1.47        | 1.39     |
| 22  | b     | 6021 | CLA  | CHC-C4B | 3.37 | 1.47        | 1.39     |
| 23  | a     | 6038 | PHO  | CBB-CAB | 3.37 | 1.50        | 1.29     |
| 22  | C     | 1029 | CLA  | CHC-C4B | 3.37 | 1.47        | 1.39     |
| 22  | D     | 1008 | CLA  | CHC-C4B | 3.37 | 1.47        | 1.39     |
| 22  | c     | 6029 | CLA  | CHC-C4B | 3.36 | 1.47        | 1.39     |
| 23  | A     | 1038 | PHO  | CBB-CAB | 3.36 | 1.50        | 1.29     |
| 22  | b     | 6009 | CLA  | CHB-C1B | 3.34 | 1.46        | 1.39     |
| 22  | B     | 1014 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | d     | 6005 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | c     | 6031 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | b     | 6014 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22  | a     | 6006 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | C     | 1037 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | d     | 6008 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | h     | 6017 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | B     | 1009 | CLA  | CHB-C1B | 3.33 | 1.46        | 1.39     |
| 22  | B     | 1019 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | b     | 6024 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | c     | 6035 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | C     | 1035 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | C     | 1027 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | B     | 1013 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | C     | 1025 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | C     | 1026 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | c     | 6027 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | D     | 1008 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | a     | 6003 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | B     | 1020 | CLA  | CHB-C1B | 3.32 | 1.46        | 1.39     |
| 22  | C     | 1031 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | b     | 6019 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | c     | 6037 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | d     | 6004 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | A     | 1007 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | A     | 1003 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | B     | 1016 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | D     | 1005 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | B     | 1010 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | c     | 6025 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | A     | 1006 | CLA  | CHB-C1B | 3.31 | 1.46        | 1.39     |
| 22  | C     | 1036 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | c     | 6026 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | C     | 1033 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | c     | 6029 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | B     | 1024 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | c     | 6036 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | c     | 6028 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | B     | 1023 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | C     | 1029 | CLA  | CHB-C1B | 3.30 | 1.46        | 1.39     |
| 22  | H     | 1017 | CLA  | CHB-C1B | 3.29 | 1.46        | 1.39     |
| 22  | c     | 6033 | CLA  | CHB-C1B | 3.29 | 1.46        | 1.39     |
| 22  | D     | 1004 | CLA  | CHB-C1B | 3.29 | 1.46        | 1.39     |
| 22  | b     | 6011 | CLA  | CHB-C1B | 3.29 | 1.46        | 1.39     |
| 22  | b     | 6020 | CLA  | CHB-C1B | 3.29 | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | b     | 6023 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 22  | C     | 1028 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 22  | b     | 6010 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 22  | b     | 6013 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 22  | b     | 6018 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 22  | B     | 1015 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 22  | B     | 1018 | CLA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 22  | K     | 1034 | CLA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 22  | C     | 1032 | CLA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 22  | b     | 6015 | CLA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 22  | b     | 6016 | CLA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 22  | a     | 6007 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 22  | B     | 1012 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 22  | c     | 6032 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 22  | B     | 1022 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 22  | B     | 1011 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 22  | b     | 6012 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 22  | k     | 6034 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 22  | C     | 1030 | CLA  | CHB-C1B | 3.26  | 1.46        | 1.39     |
| 22  | c     | 6030 | CLA  | CHB-C1B | 3.26  | 1.46        | 1.39     |
| 22  | b     | 6022 | CLA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 22  | B     | 1021 | CLA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 22  | b     | 6021 | CLA  | CHB-C1B | 3.24  | 1.46        | 1.39     |
| 31  | v     | 6041 | HEM  | FE-NA   | 3.24  | 2.05        | 1.95     |
| 31  | V     | 1041 | HEM  | FE-NC   | 3.23  | 2.05        | 1.95     |
| 31  | F     | 1040 | HEM  | FE-NC   | 3.23  | 2.05        | 1.95     |
| 31  | v     | 6041 | HEM  | FE-NC   | 3.22  | 2.05        | 1.95     |
| 31  | f     | 6040 | HEM  | FE-NC   | 3.22  | 2.05        | 1.95     |
| 31  | V     | 1041 | HEM  | FE-NA   | 3.21  | 2.05        | 1.95     |
| 31  | F     | 1040 | HEM  | FE-NA   | 3.21  | 2.05        | 1.95     |
| 31  | f     | 6040 | HEM  | FE-NA   | 3.20  | 2.05        | 1.95     |
| 23  | a     | 6038 | PHO  | O2D-CGD | -3.18 | 1.25        | 1.33     |
| 23  | A     | 1038 | PHO  | O2D-CGD | -3.17 | 1.25        | 1.33     |
| 23  | D     | 1039 | PHO  | O2D-CGD | -3.16 | 1.25        | 1.33     |
| 23  | d     | 6039 | PHO  | O2D-CGD | -3.15 | 1.25        | 1.33     |
| 22  | c     | 6036 | CLA  | C1D-C2D | 3.14  | 1.51        | 1.45     |
| 22  | b     | 6013 | CLA  | C1D-C2D | 3.14  | 1.51        | 1.45     |
| 22  | B     | 1024 | CLA  | C1D-C2D | 3.13  | 1.51        | 1.45     |
| 22  | C     | 1026 | CLA  | C1D-C2D | 3.13  | 1.51        | 1.45     |
| 22  | B     | 1019 | CLA  | C1D-C2D | 3.12  | 1.51        | 1.45     |
| 22  | d     | 6004 | CLA  | C1D-C2D | 3.12  | 1.51        | 1.45     |
| 25  | d     | 6050 | BCR  | C24-C25 | -3.12 | 1.34        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1013 | CLA  | C1D-C2D | 3.12  | 1.51        | 1.45     |
| 22  | a     | 6006 | CLA  | C1D-C2D | 3.12  | 1.51        | 1.45     |
| 22  | b     | 6024 | CLA  | C1D-C2D | 3.12  | 1.51        | 1.45     |
| 25  | D     | 1050 | BCR  | C24-C25 | -3.12 | 1.34        | 1.45     |
| 22  | C     | 1027 | CLA  | C1D-C2D | 3.11  | 1.51        | 1.45     |
| 22  | c     | 6028 | CLA  | C1D-C2D | 3.11  | 1.51        | 1.45     |
| 25  | Z     | 1053 | BCR  | C24-C25 | -3.11 | 1.34        | 1.45     |
| 22  | b     | 6019 | CLA  | C1D-C2D | 3.11  | 1.51        | 1.45     |
| 25  | z     | 6053 | BCR  | C24-C25 | -3.11 | 1.34        | 1.45     |
| 22  | a     | 6003 | CLA  | C1D-C2D | 3.11  | 1.51        | 1.45     |
| 22  | C     | 1028 | CLA  | C1D-C2D | 3.11  | 1.51        | 1.45     |
| 22  | b     | 6022 | CLA  | C1D-C2D | 3.11  | 1.51        | 1.45     |
| 22  | C     | 1036 | CLA  | C1D-C2D | 3.11  | 1.51        | 1.45     |
| 25  | k     | 6051 | BCR  | C24-C25 | -3.10 | 1.34        | 1.45     |
| 22  | C     | 1032 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 22  | C     | 1037 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 22  | h     | 6017 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 22  | B     | 1016 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 22  | c     | 6037 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 22  | D     | 1005 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 22  | b     | 6016 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 25  | b     | 6045 | BCR  | C24-C25 | -3.10 | 1.34        | 1.45     |
| 22  | c     | 6026 | CLA  | C1D-C2D | 3.10  | 1.51        | 1.45     |
| 25  | K     | 1051 | BCR  | C24-C25 | -3.09 | 1.34        | 1.45     |
| 22  | c     | 6027 | CLA  | C1D-C2D | 3.09  | 1.51        | 1.45     |
| 22  | H     | 1017 | CLA  | C1D-C2D | 3.09  | 1.51        | 1.45     |
| 25  | B     | 1045 | BCR  | C24-C25 | -3.09 | 1.34        | 1.45     |
| 22  | c     | 6031 | CLA  | C1D-C2D | 3.09  | 1.51        | 1.45     |
| 22  | D     | 1004 | CLA  | C1D-C2D | 3.09  | 1.51        | 1.45     |
| 22  | c     | 6033 | CLA  | C1D-C2D | 3.09  | 1.51        | 1.45     |
| 22  | B     | 1022 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | A     | 1003 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | b     | 6012 | CLA  | C3D-C2D | 3.08  | 1.47        | 1.39     |
| 25  | C     | 1054 | BCR  | C24-C25 | -3.08 | 1.34        | 1.45     |
| 22  | B     | 1012 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | b     | 6018 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 23  | a     | 6038 | PHO  | C3B-C4B | -3.08 | 1.38        | 1.41     |
| 22  | b     | 6014 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | d     | 6005 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | a     | 6007 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | k     | 6034 | CLA  | C3D-C2D | 3.08  | 1.47        | 1.39     |
| 22  | b     | 6012 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1007 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | C     | 1025 | CLA  | C3D-C2D | 3.08  | 1.47        | 1.39     |
| 22  | c     | 6026 | CLA  | C3D-C2D | 3.08  | 1.47        | 1.39     |
| 22  | A     | 1006 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | B     | 1018 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | C     | 1025 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 22  | b     | 6018 | CLA  | C3D-C2D | 3.08  | 1.47        | 1.39     |
| 22  | D     | 1005 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | B     | 1014 | CLA  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 22  | B     | 1015 | CLA  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 23  | D     | 1039 | PHO  | C3B-C4B | -3.07 | 1.38        | 1.41     |
| 22  | C     | 1035 | CLA  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 22  | c     | 6035 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | b     | 6015 | CLA  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 22  | c     | 6032 | CLA  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 22  | b     | 6022 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | C     | 1031 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | C     | 1036 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | C     | 1033 | CLA  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 22  | B     | 1016 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | K     | 1034 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | C     | 1026 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | a     | 6003 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | c     | 6037 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 25  | c     | 6054 | BCR  | C24-C25 | -3.07 | 1.34        | 1.45     |
| 22  | b     | 6019 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 22  | C     | 1037 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 25  | h     | 6049 | BCR  | C24-C25 | -3.06 | 1.34        | 1.45     |
| 22  | a     | 6006 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | c     | 6032 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | C     | 1032 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | c     | 6035 | CLA  | C1D-C2D | 3.06  | 1.51        | 1.45     |
| 22  | B     | 1022 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 25  | H     | 1049 | BCR  | C24-C25 | -3.06 | 1.34        | 1.45     |
| 25  | t     | 1046 | BCR  | C24-C25 | -3.06 | 1.34        | 1.45     |
| 22  | B     | 1019 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | A     | 1003 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | C     | 1031 | CLA  | C1D-C2D | 3.06  | 1.51        | 1.45     |
| 22  | b     | 6016 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | B     | 1018 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | c     | 6025 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 22  | d     | 6005 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | C     | 1033 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | B     | 1012 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | K     | 1034 | CLA  | C1D-C2D | 3.05  | 1.51        | 1.45     |
| 22  | b     | 6020 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | c     | 6036 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | B     | 1020 | CLA  | C1D-C2D | 3.05  | 1.51        | 1.45     |
| 22  | c     | 6025 | CLA  | C1D-C2D | 3.05  | 1.51        | 1.45     |
| 22  | B     | 1015 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | B     | 1020 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | A     | 1006 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | c     | 6027 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 22  | B     | 1024 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 25  | T     | 6046 | BCR  | C24-C25 | -3.05 | 1.34        | 1.45     |
| 22  | C     | 1035 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | B     | 1014 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | b     | 6015 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | d     | 6004 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | b     | 6020 | CLA  | C1D-C2D | 3.04  | 1.51        | 1.45     |
| 22  | h     | 6017 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | H     | 1017 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | C     | 1027 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | B     | 1013 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | b     | 6024 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 22  | D     | 1004 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 22  | c     | 6031 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 22  | C     | 1028 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 22  | b     | 6014 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 23  | d     | 6039 | PHO  | C3B-C4B | -3.03 | 1.38        | 1.41     |
| 22  | b     | 6013 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 22  | c     | 6028 | CLA  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 22  | A     | 1007 | CLA  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 22  | c     | 6033 | CLA  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 22  | b     | 6021 | CLA  | C1D-C2D | 3.01  | 1.51        | 1.45     |
| 22  | b     | 6010 | CLA  | C1D-C2D | 3.01  | 1.51        | 1.45     |
| 22  | B     | 1021 | CLA  | C1D-C2D | 3.01  | 1.51        | 1.45     |
| 22  | k     | 6034 | CLA  | C1D-C2D | 3.00  | 1.51        | 1.45     |
| 22  | B     | 1009 | CLA  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 22  | a     | 6007 | CLA  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 22  | c     | 6030 | CLA  | C1D-C2D | 2.99  | 1.51        | 1.45     |
| 22  | B     | 1010 | CLA  | C1D-C2D | 2.99  | 1.51        | 1.45     |
| 22  | b     | 6009 | CLA  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 22  | C     | 1030 | CLA  | C1D-C2D | 2.98  | 1.51        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | A     | 1038 | PHO  | C3B-C4B | -2.98 | 1.38        | 1.41     |
| 22  | b     | 6023 | CLA  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 22  | B     | 1023 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 22  | d     | 6008 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 22  | b     | 6021 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 22  | B     | 1021 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 22  | b     | 6010 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 22  | B     | 1010 | CLA  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 22  | B     | 1023 | CLA  | C1D-C2D | 2.95  | 1.51        | 1.45     |
| 22  | c     | 6030 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 22  | D     | 1008 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 22  | C     | 1030 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 22  | B     | 1011 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 22  | b     | 6011 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 22  | b     | 6023 | CLA  | C1D-C2D | 2.92  | 1.51        | 1.45     |
| 25  | k     | 6052 | BCR  | C24-C25 | -2.92 | 1.35        | 1.45     |
| 22  | c     | 6029 | CLA  | C3D-C2D | 2.91  | 1.46        | 1.39     |
| 22  | C     | 1029 | CLA  | C3D-C2D | 2.91  | 1.46        | 1.39     |
| 22  | B     | 1009 | CLA  | C1D-C2D | 2.91  | 1.51        | 1.45     |
| 25  | C     | 1052 | BCR  | C24-C25 | -2.90 | 1.35        | 1.45     |
| 22  | C     | 1029 | CLA  | C1D-C2D | 2.90  | 1.51        | 1.45     |
| 22  | c     | 6029 | CLA  | C1D-C2D | 2.89  | 1.51        | 1.45     |
| 22  | D     | 1008 | CLA  | C1D-C2D | 2.89  | 1.51        | 1.45     |
| 22  | d     | 6008 | CLA  | C1D-C2D | 2.89  | 1.51        | 1.45     |
| 22  | B     | 1011 | CLA  | C1D-C2D | 2.89  | 1.51        | 1.45     |
| 22  | b     | 6009 | CLA  | C1D-C2D | 2.89  | 1.51        | 1.45     |
| 22  | b     | 6011 | CLA  | C1D-C2D | 2.88  | 1.51        | 1.45     |
| 31  | f     | 6040 | HEM  | CAB-C3B | 2.84  | 1.55        | 1.47     |
| 31  | F     | 1040 | HEM  | CAB-C3B | 2.82  | 1.54        | 1.47     |
| 31  | v     | 6041 | HEM  | CAB-C3B | 2.82  | 1.54        | 1.47     |
| 31  | V     | 1041 | HEM  | CAB-C3B | 2.82  | 1.54        | 1.47     |
| 31  | v     | 6041 | HEM  | CAC-C3C | 2.81  | 1.54        | 1.47     |
| 31  | V     | 1041 | HEM  | CAC-C3C | 2.80  | 1.54        | 1.47     |
| 31  | F     | 1040 | HEM  | CAC-C3C | 2.79  | 1.54        | 1.47     |
| 25  | B     | 1047 | BCR  | C24-C25 | -2.78 | 1.35        | 1.45     |
| 25  | T     | 6048 | BCR  | C24-C25 | -2.78 | 1.35        | 1.45     |
| 25  | b     | 6047 | BCR  | C24-C25 | -2.77 | 1.35        | 1.45     |
| 25  | B     | 1048 | BCR  | C24-C25 | -2.77 | 1.35        | 1.45     |
| 25  | A     | 1044 | BCR  | C24-C25 | -2.76 | 1.35        | 1.45     |
| 31  | f     | 6040 | HEM  | CAC-C3C | 2.76  | 1.54        | 1.47     |
| 24  | a     | 6043 | PQ9  | C10-C5  | 2.76  | 1.48        | 1.35     |
| 24  | A     | 1043 | PQ9  | C10-C5  | 2.76  | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | a     | 6044 | BCR  | C24-C25 | -2.75 | 1.35        | 1.45     |
| 23  | D     | 1039 | PHO  | O2A-CGA | -2.75 | 1.25        | 1.33     |
| 24  | d     | 6042 | PQ9  | C10-C5  | 2.74  | 1.48        | 1.35     |
| 23  | d     | 6039 | PHO  | O2A-CGA | -2.74 | 1.25        | 1.33     |
| 24  | D     | 1042 | PQ9  | C10-C5  | 2.74  | 1.48        | 1.35     |
| 23  | a     | 6038 | PHO  | O2A-CGA | -2.74 | 1.25        | 1.33     |
| 23  | A     | 1038 | PHO  | O2A-CGA | -2.71 | 1.25        | 1.33     |
| 22  | b     | 6012 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | B     | 1012 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 22  | c     | 6031 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 22  | c     | 6033 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 22  | b     | 6022 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 22  | c     | 6025 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 22  | C     | 1033 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 22  | B     | 1022 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 22  | b     | 6019 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 22  | C     | 1025 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 22  | d     | 6004 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 22  | H     | 1017 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 22  | C     | 1031 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 22  | D     | 1004 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 22  | a     | 6006 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 22  | d     | 6005 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | h     | 6017 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | A     | 1006 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | B     | 1019 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | c     | 6032 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | C     | 1028 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | C     | 1032 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | A     | 1007 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 22  | C     | 1027 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | B     | 1018 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | b     | 6015 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | c     | 6030 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | B     | 1009 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | D     | 1005 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | B     | 1015 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | C     | 1037 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | B     | 1010 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | b     | 6021 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | c     | 6037 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | A     | 1003 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | c     | 6026 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | c     | 6035 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | b     | 6011 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | K     | 1034 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | B     | 1013 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | C     | 1030 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | b     | 6018 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | C     | 1035 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | c     | 6028 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | a     | 6007 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | c     | 6027 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | c     | 6036 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | B     | 1024 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | B     | 1011 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | B     | 1014 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | B     | 1016 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | C     | 1036 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | b     | 6010 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | a     | 6003 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | C     | 1026 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | b     | 6013 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | b     | 6020 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | B     | 1021 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | B     | 1020 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | b     | 6009 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 22  | b     | 6024 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 22  | k     | 6034 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 25  | k     | 6052 | BCR  | C30-C25 | -2.60 | 1.50        | 1.53     |
| 25  | C     | 1052 | BCR  | C30-C25 | -2.60 | 1.50        | 1.53     |
| 22  | b     | 6016 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 22  | d     | 6008 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | B     | 1023 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | b     | 6014 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | b     | 6023 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | D     | 1008 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 22  | c     | 6029 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 22  | C     | 1029 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 25  | T     | 6046 | BCR  | C30-C25 | -2.51 | 1.50        | 1.53     |
| 25  | t     | 1046 | BCR  | C30-C25 | -2.49 | 1.50        | 1.53     |
| 25  | T     | 6046 | BCR  | C1-C6   | -2.46 | 1.50        | 1.53     |
| 25  | D     | 1050 | BCR  | C8-C7   | -2.42 | 1.25        | 1.33     |
| 25  | h     | 6049 | BCR  | C8-C7   | -2.42 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | H     | 1049 | BCR  | C8-C7   | -2.42 | 1.25        | 1.33     |
| 25  | k     | 6052 | BCR  | C8-C7   | -2.41 | 1.25        | 1.33     |
| 25  | t     | 1046 | BCR  | C1-C6   | -2.41 | 1.50        | 1.53     |
| 25  | C     | 1052 | BCR  | C8-C7   | -2.41 | 1.25        | 1.33     |
| 25  | c     | 6054 | BCR  | C8-C7   | -2.41 | 1.25        | 1.33     |
| 25  | T     | 6048 | BCR  | C8-C7   | -2.41 | 1.25        | 1.33     |
| 22  | c     | 6031 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 25  | d     | 6050 | BCR  | C8-C7   | -2.40 | 1.25        | 1.33     |
| 25  | K     | 1051 | BCR  | C8-C7   | -2.40 | 1.26        | 1.33     |
| 25  | B     | 1047 | BCR  | C8-C7   | -2.40 | 1.26        | 1.33     |
| 25  | Z     | 1053 | BCR  | C8-C7   | -2.40 | 1.26        | 1.33     |
| 25  | k     | 6051 | BCR  | C8-C7   | -2.40 | 1.26        | 1.33     |
| 25  | C     | 1054 | BCR  | C8-C7   | -2.40 | 1.26        | 1.33     |
| 25  | b     | 6047 | BCR  | C8-C7   | -2.40 | 1.26        | 1.33     |
| 22  | C     | 1031 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 25  | B     | 1048 | BCR  | C8-C7   | -2.39 | 1.26        | 1.33     |
| 22  | b     | 6024 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 25  | b     | 6045 | BCR  | C8-C7   | -2.39 | 1.26        | 1.33     |
| 25  | B     | 1045 | BCR  | C8-C7   | -2.39 | 1.26        | 1.33     |
| 22  | b     | 6022 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 25  | z     | 6053 | BCR  | C8-C7   | -2.38 | 1.26        | 1.33     |
| 22  | C     | 1036 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 22  | B     | 1024 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 22  | C     | 1028 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 22  | B     | 1022 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 22  | c     | 6028 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 22  | b     | 6018 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 22  | c     | 6025 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 22  | c     | 6033 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | c     | 6036 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | C     | 1033 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | d     | 6005 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | b     | 6013 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | C     | 1025 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | c     | 6032 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | C     | 1037 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 22  | B     | 1018 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 22  | B     | 1012 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 22  | B     | 1013 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 22  | C     | 1032 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 22  | b     | 6012 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 22  | b     | 6014 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | c     | 6037 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 22  | A     | 1006 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 22  | C     | 1026 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 25  | A     | 1044 | BCR  | C30-C25 | -2.33 | 1.50        | 1.53     |
| 22  | A     | 1003 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 22  | D     | 1004 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 22  | b     | 6009 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 22  | a     | 6003 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | B     | 1020 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | D     | 1005 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | a     | 6006 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | B     | 1014 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | B     | 1009 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | A     | 1007 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | C     | 1027 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 22  | C     | 1035 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 22  | K     | 1034 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 25  | a     | 6044 | BCR  | C30-C25 | -2.31 | 1.50        | 1.53     |
| 22  | b     | 6020 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 22  | c     | 6035 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 23  | d     | 6039 | PHO  | C3A-C2A | -2.30 | 1.52        | 1.54     |
| 22  | B     | 1015 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | d     | 6004 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | h     | 6017 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | B     | 1019 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | B     | 1016 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | a     | 6007 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | d     | 6008 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | b     | 6015 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | C     | 1029 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 22  | b     | 6016 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 22  | c     | 6026 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 22  | c     | 6027 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 25  | t     | 1046 | BCR  | C8-C7   | -2.29 | 1.26        | 1.33     |
| 25  | T     | 6046 | BCR  | C8-C7   | -2.28 | 1.26        | 1.33     |
| 22  | k     | 6034 | CLA  | C4C-C3C | 2.28  | 1.48        | 1.45     |
| 22  | H     | 1017 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 22  | b     | 6019 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 25  | a     | 6044 | BCR  | C8-C7   | -2.27 | 1.26        | 1.33     |
| 25  | A     | 1044 | BCR  | C8-C7   | -2.27 | 1.26        | 1.33     |
| 22  | D     | 1008 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 22  | c     | 6029 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | b     | 6023 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 22  | B     | 1010 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 22  | b     | 6010 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 22  | B     | 1023 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 25  | b     | 6045 | BCR  | C30-C25 | -2.22 | 1.50        | 1.53     |
| 23  | D     | 1039 | PHO  | C3A-C2A | -2.22 | 1.52        | 1.54     |
| 23  | A     | 1038 | PHO  | C4D-ND  | -2.21 | 1.35        | 1.38     |
| 22  | c     | 6036 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 22  | B     | 1021 | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 22  | d     | 6005 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 22  | c     | 6027 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 23  | a     | 6038 | PHO  | C4D-ND  | -2.20 | 1.35        | 1.38     |
| 22  | a     | 6007 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 22  | b     | 6020 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 22  | B     | 1020 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 22  | b     | 6021 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 22  | c     | 6025 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 22  | C     | 1036 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 25  | k     | 6051 | BCR  | C1-C6   | -2.19 | 1.51        | 1.53     |
| 22  | C     | 1027 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 23  | D     | 1039 | PHO  | C4D-ND  | -2.19 | 1.35        | 1.38     |
| 22  | B     | 1012 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 25  | b     | 6047 | BCR  | C30-C25 | -2.18 | 1.51        | 1.53     |
| 25  | z     | 6053 | BCR  | C30-C25 | -2.18 | 1.51        | 1.53     |
| 22  | b     | 6012 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 23  | A     | 1038 | PHO  | C3A-C2A | -2.18 | 1.52        | 1.54     |
| 22  | c     | 6031 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 22  | k     | 6034 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 25  | B     | 1045 | BCR  | C30-C25 | -2.17 | 1.51        | 1.53     |
| 22  | C     | 1031 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 22  | B     | 1014 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 25  | z     | 6053 | BCR  | C1-C6   | -2.17 | 1.51        | 1.53     |
| 23  | d     | 6039 | PHO  | C4D-ND  | -2.17 | 1.35        | 1.38     |
| 22  | D     | 1005 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 22  | b     | 6015 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 22  | C     | 1033 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 22  | C     | 1025 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 22  | B     | 1022 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 25  | H     | 1049 | BCR  | C1-C6   | -2.16 | 1.51        | 1.53     |
| 22  | b     | 6022 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 23  | a     | 6038 | PHO  | C3A-C2A | -2.16 | 1.52        | 1.54     |
| 22  | A     | 1007 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | b     | 6013 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 22  | c     | 6026 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 25  | Z     | 1053 | BCR  | C1-C6   | -2.16 | 1.51        | 1.53     |
| 25  | B     | 1048 | BCR  | C1-C6   | -2.16 | 1.51        | 1.53     |
| 22  | b     | 6024 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 22  | C     | 1028 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 22  | K     | 1034 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 22  | c     | 6033 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 25  | B     | 1047 | BCR  | C30-C25 | -2.15 | 1.51        | 1.53     |
| 22  | A     | 1006 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | B     | 1016 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | b     | 6016 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | b     | 6019 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | B     | 1024 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | b     | 6014 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | B     | 1013 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | B     | 1011 | CLA  | MG-NA   | -2.15 | 2.01        | 2.06     |
| 22  | B     | 1015 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | b     | 6011 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 22  | b     | 6011 | CLA  | MG-NA   | -2.15 | 2.01        | 2.06     |
| 22  | C     | 1026 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 22  | c     | 6028 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 22  | b     | 6018 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 25  | B     | 1045 | BCR  | C1-C6   | -2.14 | 1.51        | 1.53     |
| 22  | d     | 6008 | CLA  | MG-NA   | -2.14 | 2.01        | 2.06     |
| 22  | C     | 1032 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 22  | c     | 6037 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 22  | h     | 6017 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 25  | T     | 6048 | BCR  | C1-C6   | -2.14 | 1.51        | 1.53     |
| 22  | C     | 1037 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 22  | B     | 1018 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 25  | K     | 1051 | BCR  | C1-C6   | -2.13 | 1.51        | 1.53     |
| 22  | B     | 1019 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | a     | 6006 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | a     | 6003 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | B     | 1021 | CLA  | MG-NA   | -2.13 | 2.01        | 2.06     |
| 22  | D     | 1004 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 25  | Z     | 1053 | BCR  | C30-C25 | -2.13 | 1.51        | 1.53     |
| 22  | c     | 6032 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 22  | H     | 1017 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 25  | h     | 6049 | BCR  | C1-C6   | -2.12 | 1.51        | 1.53     |
| 25  | k     | 6052 | BCR  | C1-C6   | -2.12 | 1.51        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | C     | 1052 | BCR  | C1-C6   | -2.12 | 1.51        | 1.53     |
| 25  | B     | 1047 | BCR  | C1-C6   | -2.12 | 1.51        | 1.53     |
| 22  | A     | 1003 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 25  | b     | 6047 | BCR  | C1-C6   | -2.11 | 1.51        | 1.53     |
| 25  | K     | 1051 | BCR  | C30-C25 | -2.11 | 1.51        | 1.53     |
| 22  | B     | 1011 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 25  | k     | 6051 | BCR  | C30-C25 | -2.11 | 1.51        | 1.53     |
| 22  | d     | 6004 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 25  | B     | 1048 | BCR  | C30-C25 | -2.11 | 1.51        | 1.53     |
| 22  | B     | 1010 | CLA  | MG-NA   | -2.11 | 2.01        | 2.06     |
| 22  | b     | 6021 | CLA  | MG-NA   | -2.11 | 2.01        | 2.06     |
| 25  | C     | 1054 | BCR  | C1-C6   | -2.11 | 1.51        | 1.53     |
| 25  | T     | 6048 | BCR  | C30-C25 | -2.11 | 1.51        | 1.53     |
| 24  | a     | 6043 | PQ9  | C3-C2   | 2.11  | 1.39        | 1.34     |
| 22  | B     | 1023 | CLA  | MG-NA   | -2.11 | 2.01        | 2.06     |
| 25  | b     | 6045 | BCR  | C1-C6   | -2.10 | 1.51        | 1.53     |
| 22  | D     | 1008 | CLA  | MG-NA   | -2.10 | 2.01        | 2.06     |
| 22  | b     | 6010 | CLA  | MG-NA   | -2.10 | 2.01        | 2.06     |
| 22  | C     | 1035 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | C     | 1030 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 24  | d     | 6042 | PQ9  | C3-C2   | 2.10  | 1.39        | 1.34     |
| 25  | D     | 1050 | BCR  | C1-C6   | -2.10 | 1.51        | 1.53     |
| 22  | c     | 6035 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | b     | 6009 | CLA  | MG-NA   | -2.09 | 2.01        | 2.06     |
| 24  | D     | 1042 | PQ9  | C3-C2   | 2.09  | 1.39        | 1.34     |
| 22  | b     | 6021 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 25  | c     | 6054 | BCR  | C1-C6   | -2.09 | 1.51        | 1.53     |
| 22  | b     | 6023 | CLA  | MG-NA   | -2.09 | 2.01        | 2.06     |
| 22  | C     | 1030 | CLA  | MG-NA   | -2.08 | 2.01        | 2.06     |
| 22  | C     | 1030 | CLA  | C4B-NB  | -2.08 | 1.35        | 1.37     |
| 22  | C     | 1029 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 25  | D     | 1050 | BCR  | C30-C25 | -2.07 | 1.51        | 1.53     |
| 25  | d     | 6050 | BCR  | C30-C25 | -2.07 | 1.51        | 1.53     |
| 24  | A     | 1043 | PQ9  | C3-C2   | 2.07  | 1.39        | 1.34     |
| 22  | c     | 6030 | CLA  | MG-NA   | -2.07 | 2.01        | 2.06     |
| 22  | c     | 6030 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 22  | B     | 1021 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | C     | 1030 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 22  | c     | 6030 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | d     | 6008 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | a     | 6003 | CLA  | MG-NA   | -2.06 | 2.01        | 2.06     |
| 22  | b     | 6023 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | c     | 6029 | CLA  | MG-NA   | -2.06 | 2.01        | 2.06     |
| 22  | c     | 6030 | CLA  | C4B-NB  | -2.06 | 1.35        | 1.37     |
| 25  | d     | 6050 | BCR  | C1-C6   | -2.06 | 1.51        | 1.53     |
| 22  | c     | 6035 | CLA  | MG-NA   | -2.06 | 2.01        | 2.06     |
| 22  | B     | 1009 | CLA  | MG-NA   | -2.06 | 2.01        | 2.06     |
| 22  | d     | 6008 | CLA  | C1B-NB  | -2.05 | 1.35        | 1.37     |
| 22  | B     | 1023 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | b     | 6024 | CLA  | MG-NA   | -2.05 | 2.01        | 2.06     |
| 22  | D     | 1008 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | b     | 6011 | CLA  | C1B-NB  | -2.04 | 1.35        | 1.37     |
| 22  | C     | 1029 | CLA  | MG-NA   | -2.04 | 2.01        | 2.06     |
| 22  | A     | 1007 | CLA  | MG-NA   | -2.04 | 2.01        | 2.06     |
| 22  | c     | 6029 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | b     | 6018 | CLA  | MG-NA   | -2.04 | 2.01        | 2.06     |
| 22  | K     | 1034 | CLA  | MG-NA   | -2.04 | 2.01        | 2.06     |
| 22  | D     | 1008 | CLA  | C4B-NB  | -2.04 | 1.35        | 1.37     |
| 22  | d     | 6008 | CLA  | C4B-NB  | -2.04 | 1.35        | 1.37     |
| 22  | b     | 6011 | CLA  | C4B-NB  | -2.03 | 1.35        | 1.37     |
| 22  | C     | 1035 | CLA  | MG-NA   | -2.03 | 2.01        | 2.06     |
| 22  | A     | 1003 | CLA  | MG-NA   | -2.03 | 2.01        | 2.06     |
| 22  | a     | 6007 | CLA  | MG-NA   | -2.03 | 2.01        | 2.06     |
| 22  | k     | 6034 | CLA  | MG-NA   | -2.03 | 2.01        | 2.06     |
| 22  | B     | 1016 | CLA  | MG-NA   | -2.03 | 2.01        | 2.06     |
| 22  | d     | 6004 | CLA  | MG-NA   | -2.03 | 2.01        | 2.06     |
| 22  | B     | 1010 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 31  | F     | 1040 | HEM  | CMD-C2D | 2.03  | 1.54        | 1.50     |
| 22  | b     | 6013 | CLA  | MG-NA   | -2.03 | 2.01        | 2.06     |
| 22  | c     | 6027 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | C     | 1027 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | B     | 1018 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | c     | 6028 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | c     | 6032 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | A     | 1006 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | B     | 1013 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | B     | 1024 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | C     | 1028 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | a     | 6006 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | C     | 1032 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 22  | b     | 6010 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | c     | 6025 | CLA  | MG-NA   | -2.02 | 2.01        | 2.06     |
| 31  | f     | 6040 | HEM  | CMA-C3A | 2.02  | 1.54        | 1.50     |
| 22  | c     | 6031 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31  | f     | 6040 | HEM  | CMD-C2D | 2.01  | 1.54        | 1.50     |
| 22  | H     | 1017 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |
| 22  | B     | 1022 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |
| 22  | C     | 1031 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |
| 22  | C     | 1025 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |
| 22  | C     | 1033 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |
| 22  | b     | 6019 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |
| 22  | B     | 1019 | CLA  | MG-NA   | -2.01 | 2.01        | 2.06     |
| 25  | h     | 6049 | BCR  | C30-C25 | -2.00 | 1.51        | 1.53     |
| 22  | B     | 1011 | CLA  | C4B-NB  | -2.00 | 1.35        | 1.37     |
| 22  | b     | 6022 | CLA  | MG-NA   | -2.00 | 2.01        | 2.06     |
| 22  | c     | 6033 | CLA  | MG-NA   | -2.00 | 2.01        | 2.06     |
| 22  | C     | 1029 | CLA  | C4B-NB  | -2.00 | 1.35        | 1.37     |
| 22  | D     | 1004 | CLA  | MG-NA   | -2.00 | 2.01        | 2.06     |
| 31  | V     | 1041 | HEM  | CMA-C3A | 2.00  | 1.54        | 1.50     |
| 31  | v     | 6041 | HEM  | CMB-C2B | 2.00  | 1.54        | 1.50     |

All (2709) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | b     | 6045 | BCR  | C16-C17-C18 | 29.28 | 168.34      | 127.28   |
| 25  | B     | 1045 | BCR  | C16-C17-C18 | 29.26 | 168.32      | 127.28   |
| 25  | T     | 6048 | BCR  | C15-C16-C17 | 26.44 | 177.62      | 123.52   |
| 25  | B     | 1048 | BCR  | C15-C16-C17 | 26.42 | 177.57      | 123.52   |
| 25  | Z     | 1053 | BCR  | C15-C16-C17 | 26.11 | 176.94      | 123.52   |
| 25  | z     | 6053 | BCR  | C15-C16-C17 | 26.10 | 176.92      | 123.52   |
| 25  | b     | 6047 | BCR  | C20-C21-C22 | 25.89 | 163.58      | 127.28   |
| 25  | B     | 1047 | BCR  | C20-C21-C22 | 25.88 | 163.57      | 127.28   |
| 25  | k     | 6052 | BCR  | C15-C16-C17 | 25.82 | 176.36      | 123.52   |
| 25  | C     | 1052 | BCR  | C15-C16-C17 | 25.80 | 176.31      | 123.52   |
| 25  | a     | 6044 | BCR  | C7-C8-C9    | 25.30 | 163.66      | 126.23   |
| 25  | A     | 1044 | BCR  | C7-C8-C9    | 25.27 | 163.62      | 126.23   |
| 25  | a     | 6044 | BCR  | C15-C16-C17 | 24.05 | 172.74      | 123.52   |
| 25  | A     | 1044 | BCR  | C15-C16-C17 | 24.04 | 172.71      | 123.52   |
| 25  | H     | 1049 | BCR  | C15-C16-C17 | 22.88 | 170.34      | 123.52   |
| 25  | h     | 6049 | BCR  | C15-C16-C17 | 22.87 | 170.32      | 123.52   |
| 25  | k     | 6052 | BCR  | C16-C15-C14 | 22.17 | 168.88      | 123.52   |
| 25  | C     | 1052 | BCR  | C16-C15-C14 | 22.14 | 168.82      | 123.52   |
| 25  | T     | 6046 | BCR  | C20-C21-C22 | 21.28 | 157.12      | 127.28   |
| 25  | t     | 1046 | BCR  | C20-C21-C22 | 21.22 | 157.04      | 127.28   |
| 25  | t     | 1046 | BCR  | C15-C16-C17 | 21.00 | 166.48      | 123.52   |
| 25  | T     | 6046 | BCR  | C15-C16-C17 | 20.98 | 166.45      | 123.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | Z     | 1053 | BCR  | C16-C15-C14 | 20.32 | 165.11      | 123.52   |
| 25  | z     | 6053 | BCR  | C16-C15-C14 | 20.31 | 165.08      | 123.52   |
| 25  | A     | 1044 | BCR  | C20-C21-C22 | 19.61 | 154.78      | 127.28   |
| 25  | a     | 6044 | BCR  | C20-C21-C22 | 19.61 | 154.78      | 127.28   |
| 25  | C     | 1052 | BCR  | C20-C21-C22 | 19.26 | 154.29      | 127.28   |
| 25  | k     | 6052 | BCR  | C20-C21-C22 | 19.26 | 154.28      | 127.28   |
| 25  | T     | 6046 | BCR  | C16-C15-C14 | 18.41 | 161.19      | 123.52   |
| 25  | t     | 1046 | BCR  | C16-C15-C14 | 18.40 | 161.16      | 123.52   |
| 25  | T     | 6046 | BCR  | C21-C20-C19 | 18.16 | 175.81      | 123.20   |
| 25  | t     | 1046 | BCR  | C21-C20-C19 | 18.15 | 175.79      | 123.20   |
| 25  | C     | 1052 | BCR  | C10-C11-C12 | 17.78 | 174.71      | 123.20   |
| 25  | k     | 6052 | BCR  | C10-C11-C12 | 17.77 | 174.69      | 123.20   |
| 25  | T     | 6048 | BCR  | C21-C20-C19 | 17.33 | 173.41      | 123.20   |
| 25  | B     | 1048 | BCR  | C21-C20-C19 | 17.33 | 173.41      | 123.20   |
| 25  | a     | 6044 | BCR  | C21-C20-C19 | 17.21 | 173.08      | 123.20   |
| 25  | A     | 1044 | BCR  | C21-C20-C19 | 17.20 | 173.04      | 123.20   |
| 25  | C     | 1054 | BCR  | C15-C16-C17 | 16.97 | 158.24      | 123.52   |
| 25  | c     | 6054 | BCR  | C15-C16-C17 | 16.95 | 158.21      | 123.52   |
| 25  | K     | 1051 | BCR  | C16-C15-C14 | 16.81 | 157.91      | 123.52   |
| 25  | k     | 6051 | BCR  | C16-C15-C14 | 16.80 | 157.90      | 123.52   |
| 25  | C     | 1052 | BCR  | C21-C20-C19 | 16.74 | 171.71      | 123.20   |
| 25  | k     | 6052 | BCR  | C21-C20-C19 | 16.73 | 171.69      | 123.20   |
| 25  | c     | 6054 | BCR  | C10-C11-C12 | 16.68 | 171.52      | 123.20   |
| 25  | C     | 1054 | BCR  | C10-C11-C12 | 16.67 | 171.50      | 123.20   |
| 25  | a     | 6044 | BCR  | C16-C17-C18 | 16.25 | 150.07      | 127.28   |
| 25  | A     | 1044 | BCR  | C16-C17-C18 | 16.25 | 150.07      | 127.28   |
| 25  | B     | 1045 | BCR  | C10-C11-C12 | 15.48 | 168.05      | 123.20   |
| 25  | B     | 1048 | BCR  | C16-C15-C14 | 15.46 | 155.16      | 123.52   |
| 25  | b     | 6045 | BCR  | C10-C11-C12 | 15.46 | 168.01      | 123.20   |
| 25  | T     | 6048 | BCR  | C16-C15-C14 | 15.46 | 155.15      | 123.52   |
| 25  | B     | 1045 | BCR  | C15-C16-C17 | 15.46 | 155.15      | 123.52   |
| 25  | b     | 6045 | BCR  | C15-C16-C17 | 15.43 | 155.08      | 123.52   |
| 25  | d     | 6050 | BCR  | C16-C15-C14 | 15.40 | 155.04      | 123.52   |
| 25  | D     | 1050 | BCR  | C16-C15-C14 | 15.37 | 154.98      | 123.52   |
| 25  | b     | 6047 | BCR  | C15-C16-C17 | 15.10 | 154.41      | 123.52   |
| 25  | B     | 1047 | BCR  | C15-C16-C17 | 15.08 | 154.38      | 123.52   |
| 25  | D     | 1050 | BCR  | C15-C16-C17 | 14.99 | 154.18      | 123.52   |
| 25  | k     | 6051 | BCR  | C15-C16-C17 | 14.99 | 154.18      | 123.52   |
| 25  | d     | 6050 | BCR  | C15-C16-C17 | 14.99 | 154.18      | 123.52   |
| 25  | K     | 1051 | BCR  | C15-C16-C17 | 14.97 | 154.14      | 123.52   |
| 25  | d     | 6050 | BCR  | C20-C21-C22 | 14.93 | 148.22      | 127.28   |
| 25  | D     | 1050 | BCR  | C20-C21-C22 | 14.90 | 148.17      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | H     | 1049 | BCR  | C16-C15-C14 | 14.64 | 153.48      | 123.52   |
| 25  | h     | 6049 | BCR  | C16-C15-C14 | 14.63 | 153.46      | 123.52   |
| 25  | c     | 6054 | BCR  | C16-C15-C14 | 14.46 | 153.11      | 123.52   |
| 25  | C     | 1054 | BCR  | C16-C15-C14 | 14.45 | 153.09      | 123.52   |
| 25  | a     | 6044 | BCR  | C16-C15-C14 | 14.31 | 152.81      | 123.52   |
| 25  | A     | 1044 | BCR  | C16-C15-C14 | 14.28 | 152.74      | 123.52   |
| 25  | c     | 6054 | BCR  | C11-C12-C13 | 13.95 | 164.62      | 126.36   |
| 25  | C     | 1054 | BCR  | C11-C12-C13 | 13.94 | 164.60      | 126.36   |
| 25  | T     | 6048 | BCR  | C20-C21-C22 | 13.20 | 145.79      | 127.28   |
| 25  | B     | 1048 | BCR  | C20-C21-C22 | 13.20 | 145.79      | 127.28   |
| 25  | k     | 6052 | BCR  | C16-C17-C18 | 12.68 | 145.06      | 127.28   |
| 25  | C     | 1052 | BCR  | C16-C17-C18 | 12.66 | 145.04      | 127.28   |
| 25  | b     | 6045 | BCR  | C7-C8-C9    | 12.66 | 144.97      | 126.23   |
| 25  | B     | 1045 | BCR  | C7-C8-C9    | 12.63 | 144.93      | 126.23   |
| 25  | A     | 1044 | BCR  | C11-C12-C13 | 12.58 | 160.85      | 126.36   |
| 25  | a     | 6044 | BCR  | C11-C12-C13 | 12.57 | 160.83      | 126.36   |
| 25  | D     | 1050 | BCR  | C11-C12-C13 | 12.52 | 160.70      | 126.36   |
| 25  | d     | 6050 | BCR  | C11-C12-C13 | 12.52 | 160.70      | 126.36   |
| 25  | z     | 6053 | BCR  | C10-C11-C12 | 12.52 | 159.48      | 123.20   |
| 25  | Z     | 1053 | BCR  | C10-C11-C12 | 12.51 | 159.45      | 123.20   |
| 25  | B     | 1048 | BCR  | C16-C17-C18 | 12.48 | 144.78      | 127.28   |
| 25  | T     | 6048 | BCR  | C16-C17-C18 | 12.44 | 144.72      | 127.28   |
| 25  | b     | 6045 | BCR  | C16-C15-C14 | 12.41 | 148.92      | 123.52   |
| 25  | B     | 1045 | BCR  | C16-C15-C14 | 12.41 | 148.92      | 123.52   |
| 25  | Z     | 1053 | BCR  | C7-C8-C9    | 12.05 | 144.06      | 126.23   |
| 25  | z     | 6053 | BCR  | C7-C8-C9    | 12.02 | 144.02      | 126.23   |
| 25  | t     | 1046 | BCR  | C16-C17-C18 | 11.80 | 143.82      | 127.28   |
| 25  | T     | 6046 | BCR  | C16-C17-C18 | 11.77 | 143.78      | 127.28   |
| 25  | d     | 6050 | BCR  | C10-C11-C12 | 11.70 | 157.10      | 123.20   |
| 25  | D     | 1050 | BCR  | C10-C11-C12 | 11.69 | 157.08      | 123.20   |
| 25  | a     | 6044 | BCR  | C10-C11-C12 | 11.51 | 156.56      | 123.20   |
| 25  | A     | 1044 | BCR  | C10-C11-C12 | 11.51 | 156.55      | 123.20   |
| 25  | h     | 6049 | BCR  | C10-C11-C12 | 11.42 | 156.29      | 123.20   |
| 25  | H     | 1049 | BCR  | C10-C11-C12 | 11.40 | 156.24      | 123.20   |
| 25  | k     | 6052 | BCR  | C11-C12-C13 | 10.92 | 156.30      | 126.36   |
| 25  | C     | 1052 | BCR  | C11-C12-C13 | 10.91 | 156.29      | 126.36   |
| 25  | k     | 6051 | BCR  | C11-C12-C13 | 10.87 | 156.17      | 126.36   |
| 25  | K     | 1051 | BCR  | C11-C12-C13 | 10.86 | 156.14      | 126.36   |
| 25  | B     | 1048 | BCR  | C20-C19-C18 | 10.81 | 156.01      | 126.36   |
| 25  | T     | 6048 | BCR  | C20-C19-C18 | 10.80 | 155.97      | 126.36   |
| 25  | d     | 6050 | BCR  | C21-C20-C19 | 10.80 | 154.49      | 123.20   |
| 25  | D     | 1050 | BCR  | C21-C20-C19 | 10.79 | 154.47      | 123.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | b     | 6047 | BCR  | C21-C20-C19 | 10.73 | 154.30      | 123.20   |
| 25  | c     | 6054 | BCR  | C21-C20-C19 | 10.73 | 154.29      | 123.20   |
| 25  | B     | 1047 | BCR  | C21-C20-C19 | 10.72 | 154.27      | 123.20   |
| 25  | C     | 1054 | BCR  | C21-C20-C19 | 10.72 | 154.27      | 123.20   |
| 25  | h     | 6049 | BCR  | C21-C20-C19 | 10.69 | 154.17      | 123.20   |
| 25  | b     | 6045 | BCR  | C21-C20-C19 | 10.69 | 154.16      | 123.20   |
| 25  | H     | 1049 | BCR  | C21-C20-C19 | 10.68 | 154.13      | 123.20   |
| 25  | B     | 1045 | BCR  | C21-C20-C19 | 10.67 | 154.11      | 123.20   |
| 25  | z     | 6053 | BCR  | C21-C20-C19 | 10.67 | 154.11      | 123.20   |
| 25  | K     | 1051 | BCR  | C21-C20-C19 | 10.66 | 154.09      | 123.20   |
| 25  | k     | 6051 | BCR  | C21-C20-C19 | 10.65 | 154.07      | 123.20   |
| 25  | Z     | 1053 | BCR  | C21-C20-C19 | 10.64 | 154.04      | 123.20   |
| 25  | k     | 6051 | BCR  | C20-C21-C22 | 10.59 | 142.12      | 127.28   |
| 25  | K     | 1051 | BCR  | C20-C21-C22 | 10.55 | 142.08      | 127.28   |
| 25  | C     | 1054 | BCR  | C16-C17-C18 | 10.46 | 141.95      | 127.28   |
| 25  | c     | 6054 | BCR  | C16-C17-C18 | 10.45 | 141.93      | 127.28   |
| 25  | H     | 1049 | BCR  | C16-C17-C18 | 10.45 | 141.93      | 127.28   |
| 25  | h     | 6049 | BCR  | C16-C17-C18 | 10.45 | 141.93      | 127.28   |
| 25  | C     | 1054 | BCR  | C20-C21-C22 | 10.40 | 141.87      | 127.28   |
| 25  | c     | 6054 | BCR  | C20-C21-C22 | 10.39 | 141.86      | 127.28   |
| 25  | H     | 1049 | BCR  | C20-C21-C22 | 10.32 | 141.75      | 127.28   |
| 25  | K     | 1051 | BCR  | C16-C17-C18 | 10.31 | 141.74      | 127.28   |
| 25  | D     | 1050 | BCR  | C16-C17-C18 | 10.31 | 141.74      | 127.28   |
| 25  | k     | 6051 | BCR  | C16-C17-C18 | 10.30 | 141.72      | 127.28   |
| 25  | d     | 6050 | BCR  | C16-C17-C18 | 10.29 | 141.71      | 127.28   |
| 25  | B     | 1047 | BCR  | C16-C17-C18 | 10.28 | 141.69      | 127.28   |
| 25  | z     | 6053 | BCR  | C16-C17-C18 | 10.28 | 141.69      | 127.28   |
| 25  | b     | 6047 | BCR  | C16-C17-C18 | 10.27 | 141.68      | 127.28   |
| 25  | Z     | 1053 | BCR  | C16-C17-C18 | 10.26 | 141.67      | 127.28   |
| 25  | h     | 6049 | BCR  | C20-C21-C22 | 10.25 | 141.66      | 127.28   |
| 25  | B     | 1045 | BCR  | C20-C21-C22 | 10.24 | 141.63      | 127.28   |
| 25  | Z     | 1053 | BCR  | C20-C21-C22 | 10.23 | 141.63      | 127.28   |
| 25  | z     | 6053 | BCR  | C20-C21-C22 | 10.21 | 141.60      | 127.28   |
| 25  | b     | 6045 | BCR  | C20-C21-C22 | 10.21 | 141.59      | 127.28   |
| 25  | k     | 6051 | BCR  | C7-C8-C9    | 10.07 | 141.13      | 126.23   |
| 25  | K     | 1051 | BCR  | C7-C8-C9    | 10.03 | 141.07      | 126.23   |
| 25  | T     | 6048 | BCR  | C7-C8-C9    | 9.95  | 140.96      | 126.23   |
| 25  | B     | 1048 | BCR  | C7-C8-C9    | 9.92  | 140.91      | 126.23   |
| 25  | B     | 1048 | BCR  | C11-C12-C13 | 9.88  | 153.45      | 126.36   |
| 25  | T     | 6048 | BCR  | C11-C12-C13 | 9.87  | 153.43      | 126.36   |
| 25  | K     | 1051 | BCR  | C10-C11-C12 | 9.77  | 151.51      | 123.20   |
| 25  | k     | 6051 | BCR  | C10-C11-C12 | 9.76  | 151.48      | 123.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | B     | 1047 | BCR  | C7-C8-C9    | 9.24  | 139.90      | 126.23   |
| 25  | b     | 6047 | BCR  | C7-C8-C9    | 9.21  | 139.86      | 126.23   |
| 25  | h     | 6049 | BCR  | C11-C12-C13 | 9.17  | 151.52      | 126.36   |
| 25  | H     | 1049 | BCR  | C11-C12-C13 | 9.15  | 151.46      | 126.36   |
| 25  | T     | 6046 | BCR  | C10-C11-C12 | 9.04  | 149.38      | 123.20   |
| 23  | a     | 6038 | PHO  | CAC-C3C-C2C | -9.04 | 110.96      | 127.56   |
| 25  | t     | 1046 | BCR  | C10-C11-C12 | 9.02  | 149.35      | 123.20   |
| 23  | A     | 1038 | PHO  | CAC-C3C-C2C | -9.02 | 110.98      | 127.56   |
| 25  | b     | 6047 | BCR  | C16-C15-C14 | 9.00  | 141.93      | 123.52   |
| 23  | d     | 6039 | PHO  | CAC-C3C-C2C | -8.99 | 111.04      | 127.56   |
| 23  | D     | 1039 | PHO  | CAC-C3C-C2C | -8.99 | 111.04      | 127.56   |
| 25  | B     | 1047 | BCR  | C16-C15-C14 | 8.99  | 141.91      | 123.52   |
| 25  | c     | 6054 | BCR  | C7-C8-C9    | 8.95  | 139.47      | 126.23   |
| 25  | C     | 1054 | BCR  | C7-C8-C9    | 8.92  | 139.44      | 126.23   |
| 25  | Z     | 1053 | BCR  | C11-C12-C13 | 8.89  | 150.74      | 126.36   |
| 25  | z     | 6053 | BCR  | C11-C12-C13 | 8.89  | 150.74      | 126.36   |
| 25  | B     | 1048 | BCR  | C10-C11-C12 | 8.80  | 148.70      | 123.20   |
| 25  | T     | 6048 | BCR  | C10-C11-C12 | 8.79  | 148.68      | 123.20   |
| 23  | D     | 1039 | PHO  | CMC-C2C-C1C | -8.48 | 109.47      | 124.73   |
| 23  | d     | 6039 | PHO  | CMC-C2C-C1C | -8.48 | 109.48      | 124.73   |
| 23  | a     | 6038 | PHO  | CMC-C2C-C1C | -8.46 | 109.52      | 124.73   |
| 23  | a     | 6038 | PHO  | C2D-C1D-ND  | 8.46  | 115.54      | 109.43   |
| 23  | A     | 1038 | PHO  | CMC-C2C-C1C | -8.45 | 109.52      | 124.73   |
| 23  | a     | 6038 | PHO  | O2D-CGD-CBD | 8.44  | 120.22      | 110.95   |
| 23  | A     | 1038 | PHO  | O2D-CGD-CBD | 8.44  | 120.22      | 110.95   |
| 23  | d     | 6039 | PHO  | C2D-C1D-ND  | 8.43  | 115.53      | 109.43   |
| 23  | D     | 1039 | PHO  | C2D-C1D-ND  | 8.43  | 115.52      | 109.43   |
| 23  | A     | 1038 | PHO  | C2D-C1D-ND  | 8.41  | 115.51      | 109.43   |
| 23  | D     | 1039 | PHO  | O2D-CGD-CBD | 8.38  | 120.15      | 110.95   |
| 23  | a     | 6038 | PHO  | CMD-C2D-C3D | -8.36 | 107.97      | 124.68   |
| 23  | A     | 1038 | PHO  | CMD-C2D-C3D | -8.36 | 107.97      | 124.68   |
| 23  | d     | 6039 | PHO  | CMD-C2D-C3D | -8.36 | 107.99      | 124.68   |
| 23  | D     | 1039 | PHO  | CMD-C2D-C3D | -8.35 | 107.99      | 124.68   |
| 23  | d     | 6039 | PHO  | O2D-CGD-CBD | 8.33  | 120.10      | 110.95   |
| 22  | d     | 6008 | CLA  | CMD-C2D-C1D | 8.28  | 139.31      | 124.73   |
| 22  | B     | 1021 | CLA  | CMD-C2D-C1D | 8.26  | 139.27      | 124.73   |
| 22  | b     | 6018 | CLA  | CMD-C2D-C1D | 8.25  | 139.26      | 124.73   |
| 22  | D     | 1008 | CLA  | CMD-C2D-C1D | 8.25  | 139.26      | 124.73   |
| 22  | C     | 1029 | CLA  | CMD-C2D-C1D | 8.25  | 139.25      | 124.73   |
| 22  | c     | 6029 | CLA  | CMD-C2D-C1D | 8.25  | 139.25      | 124.73   |
| 22  | a     | 6003 | CLA  | CMD-C2D-C1D | 8.24  | 139.25      | 124.73   |
| 22  | C     | 1030 | CLA  | CMD-C2D-C1D | 8.24  | 139.24      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | b     | 6023 | CLA  | CMD-C2D-C1D | 8.24 | 139.23      | 124.73   |
| 22  | c     | 6030 | CLA  | CMD-C2D-C1D | 8.24 | 139.23      | 124.73   |
| 22  | b     | 6021 | CLA  | CMD-C2D-C1D | 8.23 | 139.22      | 124.73   |
| 22  | c     | 6026 | CLA  | CMD-C2D-C1D | 8.22 | 139.21      | 124.73   |
| 22  | A     | 1003 | CLA  | CMD-C2D-C1D | 8.22 | 139.21      | 124.73   |
| 22  | c     | 6035 | CLA  | CMD-C2D-C1D | 8.22 | 139.21      | 124.73   |
| 22  | B     | 1018 | CLA  | CMD-C2D-C1D | 8.22 | 139.20      | 124.73   |
| 22  | C     | 1026 | CLA  | CMD-C2D-C1D | 8.22 | 139.20      | 124.73   |
| 22  | K     | 1034 | CLA  | CMD-C2D-C1D | 8.22 | 139.20      | 124.73   |
| 22  | B     | 1023 | CLA  | CMD-C2D-C1D | 8.22 | 139.20      | 124.73   |
| 22  | k     | 6034 | CLA  | CMD-C2D-C1D | 8.22 | 139.20      | 124.73   |
| 22  | b     | 6020 | CLA  | CMD-C2D-C1D | 8.21 | 139.19      | 124.73   |
| 22  | c     | 6027 | CLA  | CMD-C2D-C1D | 8.21 | 139.19      | 124.73   |
| 22  | B     | 1020 | CLA  | CMD-C2D-C1D | 8.21 | 139.19      | 124.73   |
| 22  | D     | 1005 | CLA  | CMD-C2D-C1D | 8.21 | 139.19      | 124.73   |
| 22  | C     | 1025 | CLA  | CMD-C2D-C1D | 8.21 | 139.19      | 124.73   |
| 22  | B     | 1015 | CLA  | CMD-C2D-C1D | 8.21 | 139.18      | 124.73   |
| 22  | C     | 1033 | CLA  | CMD-C2D-C1D | 8.21 | 139.18      | 124.73   |
| 22  | c     | 6025 | CLA  | CMD-C2D-C1D | 8.21 | 139.18      | 124.73   |
| 22  | C     | 1036 | CLA  | CMD-C2D-C1D | 8.20 | 139.18      | 124.73   |
| 22  | d     | 6005 | CLA  | CMD-C2D-C1D | 8.20 | 139.18      | 124.73   |
| 22  | B     | 1024 | CLA  | CMD-C2D-C1D | 8.20 | 139.18      | 124.73   |
| 22  | b     | 6012 | CLA  | CMD-C2D-C1D | 8.20 | 139.17      | 124.73   |
| 22  | b     | 6024 | CLA  | CMD-C2D-C1D | 8.20 | 139.17      | 124.73   |
| 22  | C     | 1031 | CLA  | CMD-C2D-C1D | 8.20 | 139.17      | 124.73   |
| 22  | b     | 6010 | CLA  | CMD-C2D-C1D | 8.20 | 139.17      | 124.73   |
| 22  | b     | 6015 | CLA  | CMD-C2D-C1D | 8.20 | 139.17      | 124.73   |
| 22  | c     | 6036 | CLA  | CMD-C2D-C1D | 8.20 | 139.17      | 124.73   |
| 22  | b     | 6022 | CLA  | CMD-C2D-C1D | 8.20 | 139.17      | 124.73   |
| 22  | A     | 1007 | CLA  | CMD-C2D-C1D | 8.20 | 139.16      | 124.73   |
| 22  | B     | 1016 | CLA  | CMD-C2D-C1D | 8.20 | 139.16      | 124.73   |
| 22  | B     | 1014 | CLA  | CMD-C2D-C1D | 8.20 | 139.16      | 124.73   |
| 22  | C     | 1027 | CLA  | CMD-C2D-C1D | 8.20 | 139.16      | 124.73   |
| 22  | B     | 1019 | CLA  | CMD-C2D-C1D | 8.19 | 139.16      | 124.73   |
| 22  | c     | 6031 | CLA  | CMD-C2D-C1D | 8.19 | 139.16      | 124.73   |
| 22  | C     | 1032 | CLA  | CMD-C2D-C1D | 8.19 | 139.15      | 124.73   |
| 22  | b     | 6016 | CLA  | CMD-C2D-C1D | 8.19 | 139.15      | 124.73   |
| 22  | B     | 1022 | CLA  | CMD-C2D-C1D | 8.19 | 139.15      | 124.73   |
| 22  | C     | 1035 | CLA  | CMD-C2D-C1D | 8.19 | 139.15      | 124.73   |
| 22  | b     | 6019 | CLA  | CMD-C2D-C1D | 8.19 | 139.15      | 124.73   |
| 22  | C     | 1037 | CLA  | CMD-C2D-C1D | 8.19 | 139.15      | 124.73   |
| 22  | B     | 1012 | CLA  | CMD-C2D-C1D | 8.19 | 139.15      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | d     | 6004 | CLA  | CMD-C2D-C1D | 8.18 | 139.14      | 124.73   |
| 22  | h     | 6017 | CLA  | CMD-C2D-C1D | 8.18 | 139.14      | 124.73   |
| 22  | a     | 6006 | CLA  | CMD-C2D-C1D | 8.18 | 139.14      | 124.73   |
| 22  | c     | 6033 | CLA  | CMD-C2D-C1D | 8.18 | 139.14      | 124.73   |
| 22  | D     | 1004 | CLA  | CMD-C2D-C1D | 8.18 | 139.13      | 124.73   |
| 22  | B     | 1010 | CLA  | CMD-C2D-C1D | 8.18 | 139.13      | 124.73   |
| 22  | a     | 6007 | CLA  | CMD-C2D-C1D | 8.18 | 139.13      | 124.73   |
| 22  | c     | 6037 | CLA  | CMD-C2D-C1D | 8.18 | 139.13      | 124.73   |
| 22  | C     | 1028 | CLA  | CMD-C2D-C1D | 8.17 | 139.12      | 124.73   |
| 22  | H     | 1017 | CLA  | CMD-C2D-C1D | 8.17 | 139.12      | 124.73   |
| 22  | B     | 1013 | CLA  | CMD-C2D-C1D | 8.17 | 139.12      | 124.73   |
| 25  | c     | 6054 | BCR  | C20-C19-C18 | 8.17 | 148.77      | 126.36   |
| 22  | b     | 6013 | CLA  | CMD-C2D-C1D | 8.17 | 139.12      | 124.73   |
| 22  | c     | 6032 | CLA  | CMD-C2D-C1D | 8.17 | 139.12      | 124.73   |
| 22  | A     | 1006 | CLA  | CMD-C2D-C1D | 8.17 | 139.12      | 124.73   |
| 22  | b     | 6014 | CLA  | CMD-C2D-C1D | 8.17 | 139.12      | 124.73   |
| 22  | c     | 6028 | CLA  | CMD-C2D-C1D | 8.17 | 139.11      | 124.73   |
| 25  | C     | 1054 | BCR  | C20-C19-C18 | 8.16 | 148.74      | 126.36   |
| 22  | B     | 1009 | CLA  | CMD-C2D-C1D | 8.15 | 139.08      | 124.73   |
| 22  | b     | 6009 | CLA  | CMD-C2D-C1D | 8.14 | 139.07      | 124.73   |
| 22  | B     | 1011 | CLA  | CMD-C2D-C1D | 8.11 | 139.01      | 124.73   |
| 22  | b     | 6011 | CLA  | CMD-C2D-C1D | 8.09 | 138.98      | 124.73   |
| 25  | d     | 6050 | BCR  | C7-C8-C9    | 7.80 | 137.77      | 126.23   |
| 25  | D     | 1050 | BCR  | C7-C8-C9    | 7.78 | 137.75      | 126.23   |
| 25  | H     | 1049 | BCR  | C7-C8-C9    | 7.65 | 137.56      | 126.23   |
| 25  | h     | 6049 | BCR  | C7-C8-C9    | 7.63 | 137.53      | 126.23   |
| 23  | A     | 1038 | PHO  | C2B-C1B-NB  | 7.44 | 114.81      | 109.43   |
| 23  | D     | 1039 | PHO  | C2B-C1B-NB  | 7.39 | 114.77      | 109.43   |
| 23  | d     | 6039 | PHO  | C2B-C1B-NB  | 7.38 | 114.77      | 109.43   |
| 23  | a     | 6038 | PHO  | C2B-C1B-NB  | 7.38 | 114.77      | 109.43   |
| 25  | B     | 1047 | BCR  | C10-C11-C12 | 7.35 | 144.48      | 123.20   |
| 25  | b     | 6047 | BCR  | C10-C11-C12 | 7.34 | 144.47      | 123.20   |
| 23  | a     | 6038 | PHO  | C3B-C4B-NB  | 6.47 | 111.68      | 107.46   |
| 23  | d     | 6039 | PHO  | C3B-C4B-NB  | 6.47 | 111.68      | 107.46   |
| 22  | c     | 6030 | CLA  | C2B-C1B-NB  | 6.44 | 117.00      | 110.33   |
| 22  | C     | 1030 | CLA  | C2B-C1B-NB  | 6.43 | 116.99      | 110.33   |
| 23  | D     | 1039 | PHO  | C3B-C4B-NB  | 6.42 | 111.65      | 107.46   |
| 23  | A     | 1038 | PHO  | C3B-C4B-NB  | 6.42 | 111.65      | 107.46   |
| 22  | c     | 6035 | CLA  | C2B-C1B-NB  | 6.34 | 116.90      | 110.33   |
| 22  | b     | 6014 | CLA  | C2B-C1B-NB  | 6.32 | 116.88      | 110.33   |
| 22  | b     | 6019 | CLA  | C2B-C1B-NB  | 6.32 | 116.88      | 110.33   |
| 25  | B     | 1047 | BCR  | C20-C19-C18 | 6.32 | 143.68      | 126.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | B     | 1014 | CLA  | C2B-C1B-NB  | 6.32 | 116.88      | 110.33   |
| 22  | B     | 1019 | CLA  | C2B-C1B-NB  | 6.32 | 116.88      | 110.33   |
| 22  | d     | 6004 | CLA  | C2B-C1B-NB  | 6.31 | 116.87      | 110.33   |
| 25  | b     | 6047 | BCR  | C20-C19-C18 | 6.31 | 143.67      | 126.36   |
| 22  | C     | 1026 | CLA  | C2B-C1B-NB  | 6.30 | 116.86      | 110.33   |
| 22  | B     | 1020 | CLA  | C2B-C1B-NB  | 6.30 | 116.86      | 110.33   |
| 22  | c     | 6037 | CLA  | C2B-C1B-NB  | 6.30 | 116.86      | 110.33   |
| 22  | c     | 6026 | CLA  | C2B-C1B-NB  | 6.30 | 116.86      | 110.33   |
| 22  | C     | 1025 | CLA  | C2B-C1B-NB  | 6.30 | 116.86      | 110.33   |
| 22  | C     | 1035 | CLA  | C2B-C1B-NB  | 6.30 | 116.86      | 110.33   |
| 22  | a     | 6006 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | k     | 6034 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | B     | 1016 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | d     | 6005 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | h     | 6017 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | K     | 1034 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | c     | 6027 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | B     | 1018 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | H     | 1017 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | D     | 1004 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | C     | 1036 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | C     | 1037 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | C     | 1027 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | B     | 1024 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | b     | 6009 | CLA  | C2B-C1B-NB  | 6.29 | 116.85      | 110.33   |
| 22  | A     | 1003 | CLA  | C2B-C1B-NB  | 6.29 | 116.84      | 110.33   |
| 22  | b     | 6010 | CLA  | C2B-C1B-NB  | 6.29 | 116.84      | 110.33   |
| 22  | a     | 6003 | CLA  | C2B-C1B-NB  | 6.28 | 116.84      | 110.33   |
| 22  | A     | 1006 | CLA  | C2B-C1B-NB  | 6.28 | 116.84      | 110.33   |
| 22  | A     | 1007 | CLA  | C2B-C1B-NB  | 6.28 | 116.84      | 110.33   |
| 22  | B     | 1013 | CLA  | C2B-C1B-NB  | 6.28 | 116.84      | 110.33   |
| 22  | b     | 6024 | CLA  | C2B-C1B-NB  | 6.28 | 116.84      | 110.33   |
| 22  | C     | 1032 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | C     | 1031 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | b     | 6015 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | b     | 6020 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | c     | 6028 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | b     | 6016 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | b     | 6018 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | B     | 1010 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | c     | 6031 | CLA  | C2B-C1B-NB  | 6.27 | 116.83      | 110.33   |
| 22  | D     | 1005 | CLA  | C2B-C1B-NB  | 6.26 | 116.82      | 110.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | c     | 6036 | CLA  | C2B-C1B-NB  | 6.26  | 116.82      | 110.33   |
| 22  | B     | 1015 | CLA  | C2B-C1B-NB  | 6.26  | 116.82      | 110.33   |
| 22  | b     | 6013 | CLA  | C2B-C1B-NB  | 6.26  | 116.82      | 110.33   |
| 22  | C     | 1033 | CLA  | C2B-C1B-NB  | 6.26  | 116.81      | 110.33   |
| 22  | C     | 1028 | CLA  | C2B-C1B-NB  | 6.25  | 116.81      | 110.33   |
| 22  | c     | 6032 | CLA  | C2B-C1B-NB  | 6.25  | 116.81      | 110.33   |
| 22  | a     | 6007 | CLA  | C2B-C1B-NB  | 6.25  | 116.81      | 110.33   |
| 22  | B     | 1012 | CLA  | C2B-C1B-NB  | 6.25  | 116.81      | 110.33   |
| 22  | c     | 6025 | CLA  | C2B-C1B-NB  | 6.25  | 116.81      | 110.33   |
| 22  | d     | 6008 | CLA  | C2B-C1B-NB  | 6.25  | 116.80      | 110.33   |
| 22  | D     | 1008 | CLA  | C2B-C1B-NB  | 6.24  | 116.80      | 110.33   |
| 22  | B     | 1009 | CLA  | C2B-C1B-NB  | 6.24  | 116.80      | 110.33   |
| 22  | B     | 1009 | CLA  | C2C-C1C-NC  | 6.24  | 116.53      | 109.98   |
| 22  | b     | 6009 | CLA  | C2C-C1C-NC  | 6.24  | 116.53      | 109.98   |
| 22  | B     | 1022 | CLA  | C2B-C1B-NB  | 6.24  | 116.79      | 110.33   |
| 22  | b     | 6012 | CLA  | C2B-C1B-NB  | 6.23  | 116.79      | 110.33   |
| 22  | c     | 6033 | CLA  | C2B-C1B-NB  | 6.23  | 116.79      | 110.33   |
| 22  | b     | 6022 | CLA  | C2B-C1B-NB  | 6.22  | 116.78      | 110.33   |
| 22  | b     | 6011 | CLA  | C2B-C1B-NB  | 6.20  | 116.76      | 110.33   |
| 22  | B     | 1011 | CLA  | C2B-C1B-NB  | 6.19  | 116.75      | 110.33   |
| 25  | C     | 1052 | BCR  | C30-C25-C26 | -6.17 | 114.21      | 122.64   |
| 22  | b     | 6021 | CLA  | C2B-C1B-NB  | 6.16  | 116.72      | 110.33   |
| 22  | B     | 1021 | CLA  | C2B-C1B-NB  | 6.16  | 116.71      | 110.33   |
| 22  | c     | 6029 | CLA  | C2B-C1B-NB  | 6.15  | 116.70      | 110.33   |
| 22  | C     | 1029 | CLA  | C2B-C1B-NB  | 6.14  | 116.69      | 110.33   |
| 25  | k     | 6052 | BCR  | C30-C25-C26 | -6.14 | 114.25      | 122.64   |
| 22  | B     | 1010 | CLA  | C2C-C1C-NC  | 6.11  | 116.39      | 109.98   |
| 25  | D     | 1050 | BCR  | C20-C19-C18 | 6.10  | 143.10      | 126.36   |
| 25  | d     | 6050 | BCR  | C20-C19-C18 | 6.09  | 143.07      | 126.36   |
| 22  | D     | 1008 | CLA  | C2C-C1C-NC  | 6.09  | 116.38      | 109.98   |
| 22  | b     | 6023 | CLA  | C2B-C1B-NB  | 6.09  | 116.64      | 110.33   |
| 22  | B     | 1023 | CLA  | C2B-C1B-NB  | 6.09  | 116.64      | 110.33   |
| 22  | b     | 6024 | CLA  | C2C-C1C-NC  | 6.08  | 116.37      | 109.98   |
| 22  | B     | 1024 | CLA  | C2C-C1C-NC  | 6.08  | 116.37      | 109.98   |
| 22  | b     | 6010 | CLA  | C2C-C1C-NC  | 6.08  | 116.37      | 109.98   |
| 22  | d     | 6005 | CLA  | C2C-C1C-NC  | 6.08  | 116.37      | 109.98   |
| 22  | k     | 6034 | CLA  | C2C-C1C-NC  | 6.08  | 116.37      | 109.98   |
| 22  | d     | 6008 | CLA  | C2C-C1C-NC  | 6.08  | 116.37      | 109.98   |
| 22  | D     | 1005 | CLA  | C2C-C1C-NC  | 6.08  | 116.37      | 109.98   |
| 22  | b     | 6014 | CLA  | C2C-C1C-NC  | 6.08  | 116.36      | 109.98   |
| 22  | K     | 1034 | CLA  | C2C-C1C-NC  | 6.07  | 116.36      | 109.98   |
| 22  | c     | 6029 | CLA  | C2C-C1C-NC  | 6.07  | 116.36      | 109.98   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 22  | c     | 6031 | CLA  | C2C-C1C-NC | 6.07 | 116.36      | 109.98   |
| 22  | c     | 6033 | CLA  | C2C-C1C-NC | 6.07 | 116.36      | 109.98   |
| 22  | B     | 1021 | CLA  | C2C-C1C-NC | 6.07 | 116.36      | 109.98   |
| 22  | c     | 6035 | CLA  | C2C-C1C-NC | 6.07 | 116.36      | 109.98   |
| 22  | b     | 6022 | CLA  | C2C-C1C-NC | 6.07 | 116.35      | 109.98   |
| 22  | A     | 1007 | CLA  | C2C-C1C-NC | 6.06 | 116.35      | 109.98   |
| 22  | a     | 6007 | CLA  | C2C-C1C-NC | 6.06 | 116.35      | 109.98   |
| 22  | C     | 1029 | CLA  | C2C-C1C-NC | 6.06 | 116.35      | 109.98   |
| 22  | a     | 6006 | CLA  | C2C-C1C-NC | 6.06 | 116.34      | 109.98   |
| 22  | b     | 6023 | CLA  | C2C-C1C-NC | 6.06 | 116.34      | 109.98   |
| 22  | B     | 1019 | CLA  | C2C-C1C-NC | 6.06 | 116.34      | 109.98   |
| 22  | b     | 6013 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | b     | 6021 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | b     | 6012 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | C     | 1033 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | C     | 1035 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | C     | 1025 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | C     | 1026 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | c     | 6028 | CLA  | C2C-C1C-NC | 6.05 | 116.34      | 109.98   |
| 22  | B     | 1013 | CLA  | C2C-C1C-NC | 6.05 | 116.33      | 109.98   |
| 22  | c     | 6026 | CLA  | C2C-C1C-NC | 6.05 | 116.33      | 109.98   |
| 22  | b     | 6019 | CLA  | C2C-C1C-NC | 6.05 | 116.33      | 109.98   |
| 22  | b     | 6020 | CLA  | C2C-C1C-NC | 6.04 | 116.33      | 109.98   |
| 22  | D     | 1004 | CLA  | C2C-C1C-NC | 6.04 | 116.33      | 109.98   |
| 22  | B     | 1014 | CLA  | C2C-C1C-NC | 6.04 | 116.33      | 109.98   |
| 22  | B     | 1022 | CLA  | C2C-C1C-NC | 6.04 | 116.33      | 109.98   |
| 22  | H     | 1017 | CLA  | C2C-C1C-NC | 6.04 | 116.33      | 109.98   |
| 22  | b     | 6018 | CLA  | C2C-C1C-NC | 6.04 | 116.32      | 109.98   |
| 22  | a     | 6003 | CLA  | C2C-C1C-NC | 6.04 | 116.32      | 109.98   |
| 22  | B     | 1020 | CLA  | C2C-C1C-NC | 6.04 | 116.32      | 109.98   |
| 22  | B     | 1016 | CLA  | C2C-C1C-NC | 6.04 | 116.32      | 109.98   |
| 22  | B     | 1012 | CLA  | C2C-C1C-NC | 6.03 | 116.32      | 109.98   |
| 22  | B     | 1015 | CLA  | C2C-C1C-NC | 6.03 | 116.32      | 109.98   |
| 22  | B     | 1018 | CLA  | C2C-C1C-NC | 6.03 | 116.32      | 109.98   |
| 22  | c     | 6036 | CLA  | C2C-C1C-NC | 6.03 | 116.32      | 109.98   |
| 22  | A     | 1006 | CLA  | C2C-C1C-NC | 6.03 | 116.32      | 109.98   |
| 22  | C     | 1031 | CLA  | C2C-C1C-NC | 6.03 | 116.32      | 109.98   |
| 22  | C     | 1036 | CLA  | C2C-C1C-NC | 6.03 | 116.31      | 109.98   |
| 22  | B     | 1011 | CLA  | C2C-C1C-NC | 6.02 | 116.31      | 109.98   |
| 22  | A     | 1003 | CLA  | C2C-C1C-NC | 6.02 | 116.31      | 109.98   |
| 22  | b     | 6015 | CLA  | C2C-C1C-NC | 6.02 | 116.31      | 109.98   |
| 22  | h     | 6017 | CLA  | C2C-C1C-NC | 6.02 | 116.30      | 109.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1028 | CLA  | C2C-C1C-NC  | 6.02  | 116.30      | 109.98   |
| 22  | C     | 1027 | CLA  | C2C-C1C-NC  | 6.01  | 116.30      | 109.98   |
| 22  | B     | 1023 | CLA  | C2C-C1C-NC  | 6.01  | 116.30      | 109.98   |
| 22  | c     | 6025 | CLA  | C2C-C1C-NC  | 6.01  | 116.29      | 109.98   |
| 22  | c     | 6027 | CLA  | C2C-C1C-NC  | 6.01  | 116.29      | 109.98   |
| 22  | C     | 1032 | CLA  | C2C-C1C-NC  | 6.00  | 116.28      | 109.98   |
| 22  | b     | 6011 | CLA  | C2C-C1C-NC  | 6.00  | 116.28      | 109.98   |
| 22  | d     | 6004 | CLA  | C2C-C1C-NC  | 6.00  | 116.28      | 109.98   |
| 22  | C     | 1037 | CLA  | C2C-C1C-NC  | 5.99  | 116.28      | 109.98   |
| 22  | c     | 6032 | CLA  | C2C-C1C-NC  | 5.99  | 116.28      | 109.98   |
| 22  | b     | 6016 | CLA  | C2C-C1C-NC  | 5.98  | 116.27      | 109.98   |
| 22  | C     | 1030 | CLA  | C2C-C1C-NC  | 5.97  | 116.25      | 109.98   |
| 22  | c     | 6030 | CLA  | C2C-C1C-NC  | 5.97  | 116.25      | 109.98   |
| 22  | c     | 6030 | CLA  | C3B-C2B-C1B | -5.96 | 100.14      | 107.17   |
| 22  | c     | 6037 | CLA  | C2C-C1C-NC  | 5.95  | 116.23      | 109.98   |
| 22  | C     | 1030 | CLA  | C3B-C2B-C1B | -5.93 | 100.18      | 107.17   |
| 25  | B     | 1045 | BCR  | C20-C19-C18 | 5.85  | 142.39      | 126.36   |
| 25  | b     | 6045 | BCR  | C20-C19-C18 | 5.83  | 142.34      | 126.36   |
| 22  | B     | 1010 | CLA  | C3B-C2B-C1B | -5.76 | 100.38      | 107.17   |
| 22  | b     | 6010 | CLA  | C3B-C2B-C1B | -5.75 | 100.39      | 107.17   |
| 22  | b     | 6011 | CLA  | C3B-C2B-C1B | -5.74 | 100.40      | 107.17   |
| 22  | c     | 6031 | CLA  | C3B-C2B-C1B | -5.74 | 100.41      | 107.17   |
| 22  | c     | 6035 | CLA  | C3B-C2B-C1B | -5.73 | 100.42      | 107.17   |
| 22  | d     | 6004 | CLA  | C3B-C2B-C1B | -5.73 | 100.42      | 107.17   |
| 22  | B     | 1009 | CLA  | C3B-C2B-C1B | -5.72 | 100.42      | 107.17   |
| 22  | b     | 6022 | CLA  | C3B-C2B-C1B | -5.72 | 100.42      | 107.17   |
| 22  | C     | 1025 | CLA  | C3B-C2B-C1B | -5.72 | 100.42      | 107.17   |
| 22  | c     | 6037 | CLA  | C3B-C2B-C1B | -5.72 | 100.43      | 107.17   |
| 22  | B     | 1018 | CLA  | C3B-C2B-C1B | -5.72 | 100.43      | 107.17   |
| 22  | B     | 1011 | CLA  | C3B-C2B-C1B | -5.72 | 100.43      | 107.17   |
| 22  | a     | 6006 | CLA  | C3B-C2B-C1B | -5.72 | 100.43      | 107.17   |
| 22  | d     | 6005 | CLA  | C3B-C2B-C1B | -5.71 | 100.44      | 107.17   |
| 22  | D     | 1004 | CLA  | C3B-C2B-C1B | -5.71 | 100.44      | 107.17   |
| 22  | b     | 6009 | CLA  | C3B-C2B-C1B | -5.71 | 100.44      | 107.17   |
| 22  | c     | 6026 | CLA  | C3B-C2B-C1B | -5.71 | 100.44      | 107.17   |
| 22  | C     | 1037 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |
| 22  | C     | 1033 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |
| 22  | k     | 6034 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |
| 22  | B     | 1019 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |
| 22  | C     | 1035 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |
| 22  | B     | 1022 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |
| 22  | C     | 1031 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | H     | 1017 | CLA  | C3B-C2B-C1B | -5.70 | 100.45      | 107.17   |
| 22  | B     | 1012 | CLA  | C3B-C2B-C1B | -5.70 | 100.46      | 107.17   |
| 22  | C     | 1027 | CLA  | C3B-C2B-C1B | -5.70 | 100.46      | 107.17   |
| 22  | B     | 1016 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | C     | 1026 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | K     | 1034 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | c     | 6025 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | A     | 1003 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | b     | 6019 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | C     | 1036 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | c     | 6027 | CLA  | C3B-C2B-C1B | -5.69 | 100.46      | 107.17   |
| 22  | B     | 1014 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | h     | 6017 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | A     | 1006 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | b     | 6018 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | A     | 1007 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | B     | 1013 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | B     | 1020 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | b     | 6014 | CLA  | C3B-C2B-C1B | -5.69 | 100.47      | 107.17   |
| 22  | B     | 1024 | CLA  | C3B-C2B-C1B | -5.68 | 100.47      | 107.17   |
| 22  | C     | 1028 | CLA  | C3B-C2B-C1B | -5.68 | 100.47      | 107.17   |
| 22  | c     | 6028 | CLA  | C3B-C2B-C1B | -5.67 | 100.48      | 107.17   |
| 22  | b     | 6012 | CLA  | C3B-C2B-C1B | -5.67 | 100.48      | 107.17   |
| 22  | c     | 6033 | CLA  | C3B-C2B-C1B | -5.67 | 100.48      | 107.17   |
| 22  | d     | 6008 | CLA  | C3B-C2B-C1B | -5.67 | 100.49      | 107.17   |
| 22  | b     | 6016 | CLA  | C3B-C2B-C1B | -5.67 | 100.49      | 107.17   |
| 22  | c     | 6036 | CLA  | C3B-C2B-C1B | -5.67 | 100.49      | 107.17   |
| 22  | C     | 1032 | CLA  | C3B-C2B-C1B | -5.66 | 100.49      | 107.17   |
| 23  | D     | 1039 | PHO  | CAC-C3C-C4C | -5.66 | 109.49      | 124.03   |
| 23  | a     | 6038 | PHO  | CAC-C3C-C4C | -5.66 | 109.49      | 124.03   |
| 22  | D     | 1005 | CLA  | C3B-C2B-C1B | -5.66 | 100.49      | 107.17   |
| 22  | D     | 1008 | CLA  | C3B-C2B-C1B | -5.66 | 100.50      | 107.17   |
| 22  | b     | 6024 | CLA  | C3B-C2B-C1B | -5.66 | 100.50      | 107.17   |
| 23  | A     | 1038 | PHO  | CAC-C3C-C4C | -5.66 | 109.49      | 124.03   |
| 23  | d     | 6039 | PHO  | CAC-C3C-C4C | -5.66 | 109.50      | 124.03   |
| 22  | b     | 6013 | CLA  | C3B-C2B-C1B | -5.66 | 100.50      | 107.17   |
| 22  | b     | 6015 | CLA  | C3B-C2B-C1B | -5.66 | 100.50      | 107.17   |
| 22  | b     | 6020 | CLA  | C3B-C2B-C1B | -5.65 | 100.50      | 107.17   |
| 22  | a     | 6003 | CLA  | C3B-C2B-C1B | -5.65 | 100.51      | 107.17   |
| 22  | c     | 6032 | CLA  | C3B-C2B-C1B | -5.65 | 100.51      | 107.17   |
| 22  | B     | 1015 | CLA  | C3B-C2B-C1B | -5.65 | 100.51      | 107.17   |
| 22  | a     | 6007 | CLA  | C3B-C2B-C1B | -5.65 | 100.51      | 107.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1029 | CLA  | C3B-C2B-C1B | -5.64 | 100.52      | 107.17   |
| 22  | c     | 6029 | CLA  | C3B-C2B-C1B | -5.63 | 100.53      | 107.17   |
| 22  | b     | 6021 | CLA  | C3B-C2B-C1B | -5.62 | 100.54      | 107.17   |
| 25  | B     | 1047 | BCR  | C11-C12-C13 | 5.62  | 141.78      | 126.36   |
| 25  | h     | 6049 | BCR  | C20-C19-C18 | 5.61  | 141.74      | 126.36   |
| 25  | H     | 1049 | BCR  | C20-C19-C18 | 5.61  | 141.74      | 126.36   |
| 25  | b     | 6047 | BCR  | C11-C12-C13 | 5.61  | 141.74      | 126.36   |
| 22  | B     | 1021 | CLA  | C3B-C2B-C1B | -5.60 | 100.56      | 107.17   |
| 22  | B     | 1023 | CLA  | C3B-C2B-C1B | -5.60 | 100.57      | 107.17   |
| 25  | k     | 6052 | BCR  | C20-C19-C18 | 5.60  | 141.71      | 126.36   |
| 22  | b     | 6023 | CLA  | C3B-C2B-C1B | -5.59 | 100.58      | 107.17   |
| 25  | k     | 6051 | BCR  | C20-C19-C18 | 5.59  | 141.69      | 126.36   |
| 25  | C     | 1052 | BCR  | C20-C19-C18 | 5.58  | 141.66      | 126.36   |
| 25  | K     | 1051 | BCR  | C20-C19-C18 | 5.58  | 141.66      | 126.36   |
| 25  | Z     | 1053 | BCR  | C20-C19-C18 | 5.58  | 141.66      | 126.36   |
| 25  | b     | 6045 | BCR  | C11-C12-C13 | 5.58  | 141.65      | 126.36   |
| 25  | B     | 1045 | BCR  | C11-C12-C13 | 5.57  | 141.63      | 126.36   |
| 25  | z     | 6053 | BCR  | C20-C19-C18 | 5.56  | 141.62      | 126.36   |
| 25  | T     | 6046 | BCR  | C20-C19-C18 | 5.53  | 141.54      | 126.36   |
| 31  | v     | 6041 | HEM  | C4D-ND-C1D  | 5.51  | 111.74      | 105.21   |
| 25  | t     | 1046 | BCR  | C20-C19-C18 | 5.51  | 141.46      | 126.36   |
| 31  | V     | 1041 | HEM  | C4D-ND-C1D  | 5.49  | 111.71      | 105.21   |
| 31  | f     | 6040 | HEM  | C4D-ND-C1D  | 5.49  | 111.71      | 105.21   |
| 31  | F     | 1040 | HEM  | C4D-ND-C1D  | 5.48  | 111.69      | 105.21   |
| 23  | D     | 1039 | PHO  | C4D-ND-C1D  | -5.36 | 102.45      | 108.87   |
| 23  | d     | 6039 | PHO  | C4D-ND-C1D  | -5.36 | 102.45      | 108.87   |
| 23  | a     | 6038 | PHO  | C4D-ND-C1D  | -5.34 | 102.47      | 108.87   |
| 23  | A     | 1038 | PHO  | C4D-ND-C1D  | -5.34 | 102.48      | 108.87   |
| 25  | A     | 1044 | BCR  | C20-C19-C18 | 5.29  | 140.87      | 126.36   |
| 25  | a     | 6044 | BCR  | C20-C19-C18 | 5.29  | 140.86      | 126.36   |
| 25  | T     | 6046 | BCR  | C11-C12-C13 | 5.26  | 140.79      | 126.36   |
| 25  | h     | 6049 | BCR  | C15-C14-C13 | -5.25 | 119.92      | 127.28   |
| 25  | t     | 1046 | BCR  | C11-C12-C13 | 5.24  | 140.73      | 126.36   |
| 25  | c     | 6054 | BCR  | C15-C14-C13 | -5.23 | 119.94      | 127.28   |
| 25  | C     | 1054 | BCR  | C15-C14-C13 | -5.23 | 119.95      | 127.28   |
| 25  | k     | 6051 | BCR  | C11-C10-C9  | -5.22 | 119.95      | 127.28   |
| 25  | k     | 6052 | BCR  | C11-C10-C9  | -5.22 | 119.95      | 127.28   |
| 25  | B     | 1045 | BCR  | C15-C14-C13 | -5.22 | 119.96      | 127.28   |
| 25  | C     | 1052 | BCR  | C11-C10-C9  | -5.21 | 119.97      | 127.28   |
| 25  | D     | 1050 | BCR  | C11-C10-C9  | -5.21 | 119.97      | 127.28   |
| 25  | b     | 6045 | BCR  | C15-C14-C13 | -5.21 | 119.97      | 127.28   |
| 25  | H     | 1049 | BCR  | C15-C14-C13 | -5.21 | 119.98      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | B     | 1045 | BCR  | C11-C10-C9  | -5.20 | 119.98      | 127.28   |
| 25  | Z     | 1053 | BCR  | C15-C14-C13 | -5.20 | 119.98      | 127.28   |
| 25  | z     | 6053 | BCR  | C15-C14-C13 | -5.20 | 119.98      | 127.28   |
| 25  | K     | 1051 | BCR  | C11-C10-C9  | -5.20 | 119.99      | 127.28   |
| 25  | b     | 6045 | BCR  | C11-C10-C9  | -5.20 | 119.99      | 127.28   |
| 22  | B     | 1023 | CLA  | O2D-CGD-CBD | 5.20  | 120.32      | 111.23   |
| 22  | b     | 6023 | CLA  | O2D-CGD-CBD | 5.20  | 120.32      | 111.23   |
| 25  | d     | 6050 | BCR  | C11-C10-C9  | -5.20 | 119.99      | 127.28   |
| 25  | b     | 6047 | BCR  | C15-C14-C13 | -5.19 | 119.99      | 127.28   |
| 25  | B     | 1047 | BCR  | C15-C14-C13 | -5.19 | 119.99      | 127.28   |
| 25  | Z     | 1053 | BCR  | C11-C10-C9  | -5.19 | 120.00      | 127.28   |
| 25  | b     | 6047 | BCR  | C11-C10-C9  | -5.19 | 120.00      | 127.28   |
| 25  | d     | 6050 | BCR  | C15-C14-C13 | -5.19 | 120.00      | 127.28   |
| 23  | d     | 6039 | PHO  | C3D-C4D-ND  | 5.19  | 114.36      | 107.71   |
| 25  | H     | 1049 | BCR  | C11-C10-C9  | -5.19 | 120.00      | 127.28   |
| 25  | C     | 1052 | BCR  | C15-C14-C13 | -5.18 | 120.01      | 127.28   |
| 25  | K     | 1051 | BCR  | C15-C14-C13 | -5.18 | 120.02      | 127.28   |
| 25  | T     | 6048 | BCR  | C15-C14-C13 | -5.18 | 120.02      | 127.28   |
| 25  | D     | 1050 | BCR  | C15-C14-C13 | -5.18 | 120.02      | 127.28   |
| 25  | T     | 6048 | BCR  | C11-C10-C9  | -5.18 | 120.02      | 127.28   |
| 25  | c     | 6054 | BCR  | C11-C10-C9  | -5.17 | 120.03      | 127.28   |
| 25  | B     | 1047 | BCR  | C11-C10-C9  | -5.17 | 120.03      | 127.28   |
| 25  | B     | 1048 | BCR  | C11-C10-C9  | -5.17 | 120.03      | 127.28   |
| 25  | k     | 6051 | BCR  | C15-C14-C13 | -5.17 | 120.03      | 127.28   |
| 23  | D     | 1039 | PHO  | C3D-C4D-ND  | 5.17  | 114.33      | 107.71   |
| 25  | B     | 1048 | BCR  | C15-C14-C13 | -5.17 | 120.03      | 127.28   |
| 23  | A     | 1038 | PHO  | C3D-C4D-ND  | 5.16  | 114.33      | 107.71   |
| 25  | h     | 6049 | BCR  | C11-C10-C9  | -5.16 | 120.04      | 127.28   |
| 25  | k     | 6052 | BCR  | C15-C14-C13 | -5.15 | 120.05      | 127.28   |
| 25  | z     | 6053 | BCR  | C11-C10-C9  | -5.15 | 120.06      | 127.28   |
| 25  | C     | 1054 | BCR  | C11-C10-C9  | -5.14 | 120.06      | 127.28   |
| 23  | a     | 6038 | PHO  | C3D-C4D-ND  | 5.14  | 114.30      | 107.71   |
| 22  | C     | 1037 | CLA  | O2D-CGD-CBD | 5.07  | 120.10      | 111.23   |
| 22  | c     | 6031 | CLA  | O2D-CGD-CBD | 5.07  | 120.10      | 111.23   |
| 22  | A     | 1003 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | c     | 6037 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | C     | 1028 | CLA  | O2D-CGD-CBD | 5.06  | 120.08      | 111.23   |
| 22  | h     | 6017 | CLA  | O2D-CGD-CBD | 5.06  | 120.08      | 111.23   |
| 22  | c     | 6028 | CLA  | O2D-CGD-CBD | 5.06  | 120.08      | 111.23   |
| 22  | a     | 6003 | CLA  | O2D-CGD-CBD | 5.06  | 120.07      | 111.23   |
| 22  | H     | 1017 | CLA  | O2D-CGD-CBD | 5.05  | 120.07      | 111.23   |
| 22  | b     | 6015 | CLA  | O2D-CGD-CBD | 5.05  | 120.06      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | B     | 1015 | CLA  | O2D-CGD-CBD | 5.05 | 120.05      | 111.23   |
| 22  | B     | 1012 | CLA  | O2D-CGD-CBD | 5.05 | 120.05      | 111.23   |
| 22  | C     | 1031 | CLA  | O2D-CGD-CBD | 5.05 | 120.05      | 111.23   |
| 22  | c     | 6035 | CLA  | O2D-CGD-CBD | 5.04 | 120.05      | 111.23   |
| 22  | a     | 6006 | CLA  | O2D-CGD-CBD | 5.04 | 120.05      | 111.23   |
| 22  | a     | 6007 | CLA  | O2D-CGD-CBD | 5.04 | 120.04      | 111.23   |
| 22  | A     | 1006 | CLA  | O2D-CGD-CBD | 5.04 | 120.03      | 111.23   |
| 22  | B     | 1014 | CLA  | O2D-CGD-CBD | 5.04 | 120.03      | 111.23   |
| 22  | b     | 6012 | CLA  | O2D-CGD-CBD | 5.03 | 120.03      | 111.23   |
| 22  | B     | 1013 | CLA  | O2D-CGD-CBD | 5.03 | 120.02      | 111.23   |
| 22  | c     | 6025 | CLA  | O2D-CGD-CBD | 5.03 | 120.02      | 111.23   |
| 22  | C     | 1027 | CLA  | O2D-CGD-CBD | 5.03 | 120.02      | 111.23   |
| 22  | b     | 6013 | CLA  | O2D-CGD-CBD | 5.02 | 120.01      | 111.23   |
| 22  | b     | 6019 | CLA  | O2D-CGD-CBD | 5.02 | 120.01      | 111.23   |
| 22  | d     | 6004 | CLA  | O2D-CGD-CBD | 5.02 | 120.01      | 111.23   |
| 22  | b     | 6020 | CLA  | O2D-CGD-CBD | 5.02 | 120.01      | 111.23   |
| 22  | A     | 1007 | CLA  | O2D-CGD-CBD | 5.02 | 120.00      | 111.23   |
| 22  | C     | 1035 | CLA  | O2D-CGD-CBD | 5.02 | 120.00      | 111.23   |
| 22  | b     | 6014 | CLA  | O2D-CGD-CBD | 5.02 | 120.00      | 111.23   |
| 22  | B     | 1019 | CLA  | O2D-CGD-CBD | 5.02 | 120.00      | 111.23   |
| 22  | C     | 1025 | CLA  | O2D-CGD-CBD | 5.01 | 120.00      | 111.23   |
| 22  | C     | 1026 | CLA  | O2D-CGD-CBD | 5.01 | 119.99      | 111.23   |
| 22  | D     | 1004 | CLA  | O2D-CGD-CBD | 5.01 | 119.99      | 111.23   |
| 22  | c     | 6026 | CLA  | O2D-CGD-CBD | 5.01 | 119.99      | 111.23   |
| 22  | B     | 1024 | CLA  | O2D-CGD-CBD | 5.01 | 119.98      | 111.23   |
| 22  | B     | 1022 | CLA  | O2D-CGD-CBD | 5.00 | 119.98      | 111.23   |
| 22  | b     | 6018 | CLA  | O2D-CGD-CBD | 5.00 | 119.98      | 111.23   |
| 22  | B     | 1020 | CLA  | O2D-CGD-CBD | 5.00 | 119.97      | 111.23   |
| 22  | B     | 1016 | CLA  | O2D-CGD-CBD | 5.00 | 119.97      | 111.23   |
| 22  | C     | 1033 | CLA  | O2D-CGD-CBD | 5.00 | 119.97      | 111.23   |
| 22  | b     | 6024 | CLA  | O2D-CGD-CBD | 5.00 | 119.97      | 111.23   |
| 22  | c     | 6027 | CLA  | O2D-CGD-CBD | 5.00 | 119.97      | 111.23   |
| 22  | C     | 1032 | CLA  | O2D-CGD-CBD | 5.00 | 119.97      | 111.23   |
| 22  | c     | 6036 | CLA  | O2D-CGD-CBD | 5.00 | 119.96      | 111.23   |
| 22  | d     | 6005 | CLA  | O2D-CGD-CBD | 4.99 | 119.96      | 111.23   |
| 22  | B     | 1018 | CLA  | O2D-CGD-CBD | 4.99 | 119.96      | 111.23   |
| 22  | b     | 6022 | CLA  | O2D-CGD-CBD | 4.99 | 119.96      | 111.23   |
| 22  | C     | 1036 | CLA  | O2D-CGD-CBD | 4.99 | 119.95      | 111.23   |
| 22  | c     | 6033 | CLA  | O2D-CGD-CBD | 4.99 | 119.94      | 111.23   |
| 22  | D     | 1005 | CLA  | O2D-CGD-CBD | 4.98 | 119.94      | 111.23   |
| 22  | b     | 6016 | CLA  | O2D-CGD-CBD | 4.97 | 119.92      | 111.23   |
| 22  | c     | 6032 | CLA  | O2D-CGD-CBD | 4.97 | 119.92      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | K     | 1034 | CLA  | O2D-CGD-CBD | 4.97  | 119.92      | 111.23   |
| 22  | b     | 6021 | CLA  | O2D-CGD-CBD | 4.97  | 119.92      | 111.23   |
| 22  | B     | 1021 | CLA  | O2D-CGD-CBD | 4.96  | 119.91      | 111.23   |
| 22  | k     | 6034 | CLA  | O2D-CGD-CBD | 4.96  | 119.91      | 111.23   |
| 22  | B     | 1010 | CLA  | O2D-CGD-CBD | 4.94  | 119.87      | 111.23   |
| 22  | b     | 6010 | CLA  | O2D-CGD-CBD | 4.92  | 119.82      | 111.23   |
| 23  | A     | 1038 | PHO  | OBD-CAD-C3D | -4.74 | 120.49      | 127.89   |
| 23  | D     | 1039 | PHO  | OBD-CAD-C3D | -4.74 | 120.49      | 127.89   |
| 23  | d     | 6039 | PHO  | OBD-CAD-C3D | -4.73 | 120.51      | 127.89   |
| 25  | t     | 1046 | BCR  | C15-C14-C13 | -4.73 | 120.64      | 127.28   |
| 23  | a     | 6038 | PHO  | OBD-CAD-C3D | -4.73 | 120.52      | 127.89   |
| 25  | T     | 6046 | BCR  | C15-C14-C13 | -4.72 | 120.67      | 127.28   |
| 22  | c     | 6030 | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 25  | A     | 1044 | BCR  | C30-C25-C26 | -4.63 | 116.31      | 122.64   |
| 25  | a     | 6044 | BCR  | C11-C10-C9  | -4.63 | 120.79      | 127.28   |
| 25  | T     | 6046 | BCR  | C11-C10-C9  | -4.63 | 120.79      | 127.28   |
| 25  | a     | 6044 | BCR  | C30-C25-C26 | -4.62 | 116.32      | 122.64   |
| 25  | C     | 1052 | BCR  | C28-C27-C26 | -4.62 | 105.81      | 114.06   |
| 25  | t     | 1046 | BCR  | C11-C10-C9  | -4.62 | 120.80      | 127.28   |
| 25  | k     | 6052 | BCR  | C28-C27-C26 | -4.62 | 105.82      | 114.06   |
| 22  | C     | 1030 | CLA  | C3D-C2D-C1D | -4.62 | 99.53       | 105.83   |
| 25  | A     | 1044 | BCR  | C11-C10-C9  | -4.59 | 120.84      | 127.28   |
| 22  | b     | 6010 | CLA  | C3D-C2D-C1D | -4.58 | 99.59       | 105.83   |
| 25  | C     | 1052 | BCR  | C27-C26-C25 | -4.58 | 116.52      | 122.70   |
| 22  | c     | 6036 | CLA  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 22  | B     | 1010 | CLA  | C3D-C2D-C1D | -4.57 | 99.60       | 105.83   |
| 25  | k     | 6052 | BCR  | C27-C26-C25 | -4.57 | 116.53      | 122.70   |
| 22  | b     | 6018 | CLA  | C3D-C2D-C1D | -4.56 | 99.60       | 105.83   |
| 22  | C     | 1036 | CLA  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 22  | d     | 6004 | CLA  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 22  | a     | 6003 | CLA  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 22  | c     | 6027 | CLA  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 22  | B     | 1018 | CLA  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 22  | b     | 6011 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 22  | B     | 1011 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 22  | b     | 6020 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 22  | C     | 1037 | CLA  | C3D-C2D-C1D | -4.53 | 99.64       | 105.83   |
| 22  | B     | 1023 | CLA  | C3D-C2D-C1D | -4.53 | 99.64       | 105.83   |
| 22  | b     | 6016 | CLA  | C3D-C2D-C1D | -4.53 | 99.64       | 105.83   |
| 22  | b     | 6020 | CLA  | CHD-C1D-ND  | -4.53 | 118.42      | 124.80   |
| 22  | B     | 1019 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | C     | 1032 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | D     | 1005 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | b     | 6023 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | h     | 6017 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | D     | 1004 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | B     | 1016 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | C     | 1025 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | C     | 1026 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | b     | 6012 | CLA  | C3D-C2D-C1D | -4.53 | 99.66       | 105.83   |
| 22  | C     | 1027 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 22  | c     | 6025 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 22  | b     | 6012 | CLA  | CHD-C1D-ND  | -4.52 | 118.44      | 124.80   |
| 22  | d     | 6008 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 22  | B     | 1012 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 22  | B     | 1021 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 22  | C     | 1031 | CLA  | C3D-C2D-C1D | -4.52 | 99.67       | 105.83   |
| 22  | B     | 1014 | CLA  | C3D-C2D-C1D | -4.52 | 99.67       | 105.83   |
| 22  | B     | 1020 | CLA  | C3D-C2D-C1D | -4.52 | 99.67       | 105.83   |
| 22  | K     | 1034 | CLA  | C3D-C2D-C1D | -4.52 | 99.67       | 105.83   |
| 22  | b     | 6013 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | c     | 6037 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | d     | 6005 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | c     | 6031 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | b     | 6022 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | b     | 6016 | CLA  | CHD-C1D-ND  | -4.51 | 118.45      | 124.80   |
| 22  | a     | 6007 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | A     | 1003 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | B     | 1024 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 22  | A     | 1007 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 22  | b     | 6019 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 22  | B     | 1015 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 22  | k     | 6034 | CLA  | CHD-C1D-ND  | -4.51 | 118.46      | 124.80   |
| 22  | b     | 6015 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 22  | b     | 6023 | CLA  | CHD-C1D-ND  | -4.51 | 118.46      | 124.80   |
| 22  | c     | 6026 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 22  | B     | 1012 | CLA  | CHD-C1D-ND  | -4.50 | 118.47      | 124.80   |
| 22  | B     | 1022 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 22  | c     | 6035 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 22  | b     | 6021 | CLA  | CHD-C1D-ND  | -4.50 | 118.47      | 124.80   |
| 22  | a     | 6006 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 22  | b     | 6014 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 22  | C     | 1033 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 22  | A     | 1006 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1023 | CLA  | CHD-C1D-ND  | -4.50 | 118.47      | 124.80   |
| 22  | C     | 1028 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 22  | C     | 1033 | CLA  | CHD-C1D-ND  | -4.50 | 118.47      | 124.80   |
| 22  | b     | 6024 | CLA  | C3D-C2D-C1D | -4.50 | 99.70       | 105.83   |
| 22  | b     | 6021 | CLA  | C3D-C2D-C1D | -4.49 | 99.70       | 105.83   |
| 22  | C     | 1035 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | b     | 6015 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | A     | 1003 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | B     | 1018 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | c     | 6032 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | B     | 1020 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | H     | 1017 | CLA  | C3D-C2D-C1D | -4.49 | 99.70       | 105.83   |
| 22  | A     | 1006 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | a     | 6006 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 22  | c     | 6028 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 22  | c     | 6025 | CLA  | CHD-C1D-ND  | -4.49 | 118.49      | 124.80   |
| 22  | C     | 1035 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 22  | C     | 1029 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 22  | A     | 1007 | CLA  | CHD-C1D-ND  | -4.49 | 118.49      | 124.80   |
| 22  | K     | 1034 | CLA  | CHD-C1D-ND  | -4.49 | 118.49      | 124.80   |
| 22  | B     | 1021 | CLA  | CHD-C1D-ND  | -4.49 | 118.49      | 124.80   |
| 22  | a     | 6007 | CLA  | CHD-C1D-ND  | -4.48 | 118.49      | 124.80   |
| 22  | D     | 1008 | CLA  | C3D-C2D-C1D | -4.48 | 99.71       | 105.83   |
| 22  | B     | 1015 | CLA  | CHD-C1D-ND  | -4.48 | 118.49      | 124.80   |
| 22  | C     | 1036 | CLA  | CHD-C1D-ND  | -4.48 | 118.49      | 124.80   |
| 22  | B     | 1013 | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 22  | B     | 1014 | CLA  | CHD-C1D-ND  | -4.48 | 118.50      | 124.80   |
| 22  | c     | 6036 | CLA  | CHD-C1D-ND  | -4.48 | 118.50      | 124.80   |
| 22  | c     | 6032 | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 22  | k     | 6034 | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 22  | c     | 6033 | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 22  | D     | 1005 | CLA  | CHD-C1D-ND  | -4.48 | 118.50      | 124.80   |
| 22  | c     | 6027 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | b     | 6014 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | c     | 6035 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | d     | 6004 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | C     | 1031 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | C     | 1032 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | d     | 6005 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | h     | 6017 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | c     | 6029 | CLA  | C3D-C2D-C1D | -4.47 | 99.73       | 105.83   |
| 22  | B     | 1016 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6018 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | D     | 1004 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | a     | 6003 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | b     | 6019 | CLA  | CHD-C1D-ND  | -4.47 | 118.51      | 124.80   |
| 22  | B     | 1009 | CLA  | C3D-C2D-C1D | -4.47 | 99.73       | 105.83   |
| 22  | B     | 1019 | CLA  | CHD-C1D-ND  | -4.47 | 118.52      | 124.80   |
| 22  | c     | 6033 | CLA  | CHD-C1D-ND  | -4.47 | 118.52      | 124.80   |
| 22  | C     | 1025 | CLA  | CHD-C1D-ND  | -4.46 | 118.52      | 124.80   |
| 22  | H     | 1017 | CLA  | CHD-C1D-ND  | -4.46 | 118.52      | 124.80   |
| 22  | B     | 1022 | CLA  | CHD-C1D-ND  | -4.46 | 118.52      | 124.80   |
| 22  | c     | 6026 | CLA  | CHD-C1D-ND  | -4.46 | 118.52      | 124.80   |
| 22  | C     | 1026 | CLA  | CHD-C1D-ND  | -4.46 | 118.53      | 124.80   |
| 22  | C     | 1027 | CLA  | CHD-C1D-ND  | -4.46 | 118.53      | 124.80   |
| 22  | B     | 1024 | CLA  | CHD-C1D-ND  | -4.45 | 118.53      | 124.80   |
| 22  | c     | 6031 | CLA  | CHD-C1D-ND  | -4.45 | 118.53      | 124.80   |
| 22  | b     | 6009 | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |
| 22  | b     | 6013 | CLA  | CHD-C1D-ND  | -4.45 | 118.54      | 124.80   |
| 22  | C     | 1028 | CLA  | CHD-C1D-ND  | -4.45 | 118.54      | 124.80   |
| 22  | C     | 1037 | CLA  | CHD-C1D-ND  | -4.44 | 118.55      | 124.80   |
| 22  | c     | 6028 | CLA  | CHD-C1D-ND  | -4.44 | 118.55      | 124.80   |
| 22  | B     | 1013 | CLA  | CHD-C1D-ND  | -4.44 | 118.56      | 124.80   |
| 22  | B     | 1010 | CLA  | CHD-C1D-ND  | -4.43 | 118.56      | 124.80   |
| 22  | c     | 6029 | CLA  | CHD-C1D-ND  | -4.43 | 118.57      | 124.80   |
| 22  | c     | 6037 | CLA  | CHD-C1D-ND  | -4.43 | 118.57      | 124.80   |
| 22  | b     | 6022 | CLA  | CHD-C1D-ND  | -4.43 | 118.57      | 124.80   |
| 22  | b     | 6024 | CLA  | CHD-C1D-ND  | -4.42 | 118.58      | 124.80   |
| 22  | c     | 6030 | CLA  | CHD-C1D-ND  | -4.42 | 118.58      | 124.80   |
| 22  | C     | 1029 | CLA  | CHD-C1D-ND  | -4.42 | 118.58      | 124.80   |
| 22  | C     | 1030 | CLA  | CHD-C1D-ND  | -4.42 | 118.59      | 124.80   |
| 22  | b     | 6010 | CLA  | CHD-C1D-ND  | -4.39 | 118.62      | 124.80   |
| 25  | C     | 1052 | BCR  | C7-C8-C9    | 4.39  | 132.74      | 126.23   |
| 25  | k     | 6052 | BCR  | C7-C8-C9    | 4.39  | 132.74      | 126.23   |
| 22  | b     | 6011 | CLA  | CHD-C1D-ND  | -4.37 | 118.65      | 124.80   |
| 22  | d     | 6008 | CLA  | CHD-C1D-ND  | -4.36 | 118.67      | 124.80   |
| 22  | b     | 6009 | CLA  | CHD-C1D-ND  | -4.35 | 118.68      | 124.80   |
| 23  | a     | 6038 | PHO  | C4B-NB-C1B  | -4.35 | 102.48      | 108.82   |
| 22  | D     | 1008 | CLA  | CHD-C1D-ND  | -4.35 | 118.69      | 124.80   |
| 22  | B     | 1011 | CLA  | CHD-C1D-ND  | -4.34 | 118.69      | 124.80   |
| 22  | B     | 1009 | CLA  | CHD-C1D-ND  | -4.34 | 118.69      | 124.80   |
| 23  | A     | 1038 | PHO  | C4B-NB-C1B  | -4.34 | 102.50      | 108.82   |
| 22  | C     | 1029 | CLA  | O2D-CGD-CBD | 4.34  | 118.81      | 111.23   |
| 22  | c     | 6029 | CLA  | O2D-CGD-CBD | 4.32  | 118.78      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | D     | 1039 | PHO  | C4B-NB-C1B  | -4.31 | 102.53      | 108.82   |
| 23  | d     | 6039 | PHO  | C4B-NB-C1B  | -4.31 | 102.53      | 108.82   |
| 25  | b     | 6047 | BCR  | C24-C23-C22 | 4.29  | 132.59      | 126.23   |
| 25  | a     | 6044 | BCR  | C24-C23-C22 | 4.28  | 132.57      | 126.23   |
| 25  | B     | 1047 | BCR  | C30-C25-C26 | -4.28 | 116.79      | 122.64   |
| 25  | b     | 6047 | BCR  | C30-C25-C26 | -4.27 | 116.80      | 122.64   |
| 25  | B     | 1048 | BCR  | C30-C25-C26 | -4.27 | 116.80      | 122.64   |
| 25  | A     | 1044 | BCR  | C24-C23-C22 | 4.27  | 132.55      | 126.23   |
| 25  | T     | 6048 | BCR  | C30-C25-C26 | -4.26 | 116.81      | 122.64   |
| 25  | B     | 1047 | BCR  | C24-C23-C22 | 4.26  | 132.53      | 126.23   |
| 25  | B     | 1048 | BCR  | C24-C23-C22 | 4.25  | 132.53      | 126.23   |
| 25  | c     | 6054 | BCR  | C24-C23-C22 | -4.25 | 119.95      | 126.23   |
| 25  | k     | 6051 | BCR  | C24-C23-C22 | -4.25 | 119.95      | 126.23   |
| 25  | T     | 6046 | BCR  | C24-C23-C22 | -4.24 | 119.96      | 126.23   |
| 25  | h     | 6049 | BCR  | C24-C23-C22 | -4.24 | 119.96      | 126.23   |
| 25  | T     | 6048 | BCR  | C24-C23-C22 | 4.24  | 132.50      | 126.23   |
| 25  | C     | 1054 | BCR  | C24-C23-C22 | -4.24 | 119.97      | 126.23   |
| 25  | h     | 6049 | BCR  | C38-C26-C25 | -4.24 | 119.86      | 124.48   |
| 25  | H     | 1049 | BCR  | C24-C23-C22 | -4.23 | 119.97      | 126.23   |
| 25  | K     | 1051 | BCR  | C24-C23-C22 | -4.23 | 119.97      | 126.23   |
| 25  | t     | 1046 | BCR  | C24-C23-C22 | -4.23 | 119.97      | 126.23   |
| 22  | b     | 6021 | CLA  | C1C-C2C-C3C | -4.22 | 102.54      | 106.98   |
| 25  | D     | 1050 | BCR  | C24-C23-C22 | -4.22 | 120.00      | 126.23   |
| 22  | B     | 1009 | CLA  | O2D-CGD-CBD | 4.21  | 118.60      | 111.23   |
| 22  | B     | 1021 | CLA  | C1C-C2C-C3C | -4.21 | 102.55      | 106.98   |
| 25  | H     | 1049 | BCR  | C38-C26-C25 | -4.21 | 119.89      | 124.48   |
| 25  | z     | 6053 | BCR  | C24-C23-C22 | -4.21 | 120.01      | 126.23   |
| 25  | Z     | 1053 | BCR  | C24-C23-C22 | -4.20 | 120.02      | 126.23   |
| 22  | b     | 6009 | CLA  | O2D-CGD-CBD | 4.20  | 118.58      | 111.23   |
| 22  | b     | 6011 | CLA  | C3C-C4C-NC  | 4.19  | 115.80      | 110.43   |
| 25  | B     | 1045 | BCR  | C24-C23-C22 | -4.19 | 120.03      | 126.23   |
| 25  | B     | 1047 | BCR  | C37-C22-C23 | 4.19  | 124.49      | 118.09   |
| 25  | b     | 6045 | BCR  | C24-C23-C22 | -4.19 | 120.03      | 126.23   |
| 25  | b     | 6045 | BCR  | C33-C5-C6   | -4.19 | 119.91      | 124.48   |
| 25  | C     | 1054 | BCR  | C38-C26-C25 | -4.19 | 119.92      | 124.48   |
| 25  | B     | 1048 | BCR  | C37-C22-C23 | 4.19  | 124.48      | 118.09   |
| 22  | B     | 1011 | CLA  | C3C-C4C-NC  | 4.18  | 115.79      | 110.43   |
| 22  | B     | 1009 | CLA  | C1C-C2C-C3C | -4.18 | 102.58      | 106.98   |
| 25  | T     | 6048 | BCR  | C37-C22-C23 | 4.18  | 124.47      | 118.09   |
| 25  | d     | 6050 | BCR  | C38-C26-C25 | -4.17 | 119.93      | 124.48   |
| 25  | b     | 6047 | BCR  | C37-C22-C23 | 4.17  | 124.46      | 118.09   |
| 22  | k     | 6034 | CLA  | C1C-C2C-C3C | -4.17 | 102.59      | 106.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | a     | 6007 | CLA  | C1C-C2C-C3C | -4.17 | 102.59      | 106.98   |
| 25  | d     | 6050 | BCR  | C24-C23-C22 | -4.17 | 120.07      | 126.23   |
| 22  | b     | 6009 | CLA  | C1C-C2C-C3C | -4.17 | 102.60      | 106.98   |
| 22  | d     | 6008 | CLA  | C3B-C4B-NB  | 4.16  | 114.25      | 110.53   |
| 25  | B     | 1045 | BCR  | C33-C5-C6   | -4.16 | 119.94      | 124.48   |
| 25  | c     | 6054 | BCR  | C38-C26-C25 | -4.16 | 119.95      | 124.48   |
| 22  | A     | 1007 | CLA  | C1C-C2C-C3C | -4.14 | 102.62      | 106.98   |
| 25  | H     | 1049 | BCR  | C33-C5-C6   | -4.14 | 119.96      | 124.48   |
| 25  | D     | 1050 | BCR  | C38-C26-C25 | -4.14 | 119.96      | 124.48   |
| 25  | k     | 6052 | BCR  | C33-C5-C6   | -4.14 | 119.96      | 124.48   |
| 25  | k     | 6051 | BCR  | C33-C5-C6   | -4.14 | 119.97      | 124.48   |
| 25  | K     | 1051 | BCR  | C38-C26-C25 | -4.14 | 119.97      | 124.48   |
| 25  | h     | 6049 | BCR  | C33-C5-C6   | -4.14 | 119.97      | 124.48   |
| 25  | k     | 6051 | BCR  | C38-C26-C25 | -4.14 | 119.97      | 124.48   |
| 25  | K     | 1051 | BCR  | C33-C5-C6   | -4.14 | 119.97      | 124.48   |
| 22  | D     | 1008 | CLA  | C3B-C4B-NB  | 4.13  | 114.22      | 110.53   |
| 25  | B     | 1047 | BCR  | C33-C5-C6   | -4.13 | 119.97      | 124.48   |
| 22  | b     | 6012 | CLA  | C1C-C2C-C3C | -4.13 | 102.63      | 106.98   |
| 22  | K     | 1034 | CLA  | C1C-C2C-C3C | -4.13 | 102.64      | 106.98   |
| 22  | b     | 6023 | CLA  | C1C-C2C-C3C | -4.13 | 102.64      | 106.98   |
| 25  | b     | 6045 | BCR  | C38-C26-C25 | -4.13 | 119.98      | 124.48   |
| 22  | b     | 6015 | CLA  | C3C-C4C-NC  | 4.13  | 115.72      | 110.43   |
| 22  | D     | 1005 | CLA  | C1C-C2C-C3C | -4.13 | 102.64      | 106.98   |
| 25  | Z     | 1053 | BCR  | C38-C26-C25 | -4.13 | 119.98      | 124.48   |
| 22  | c     | 6027 | CLA  | C1C-C2C-C3C | -4.13 | 102.64      | 106.98   |
| 22  | b     | 6014 | CLA  | C1C-C2C-C3C | -4.12 | 102.64      | 106.98   |
| 22  | d     | 6005 | CLA  | C1C-C2C-C3C | -4.12 | 102.64      | 106.98   |
| 22  | B     | 1012 | CLA  | C1C-C2C-C3C | -4.12 | 102.64      | 106.98   |
| 22  | C     | 1030 | CLA  | C1C-C2C-C3C | -4.12 | 102.64      | 106.98   |
| 22  | C     | 1030 | CLA  | C3C-C4C-NC  | 4.12  | 115.71      | 110.43   |
| 22  | c     | 6031 | CLA  | C1C-C2C-C3C | -4.12 | 102.65      | 106.98   |
| 22  | D     | 1008 | CLA  | C1C-C2C-C3C | -4.12 | 102.65      | 106.98   |
| 22  | d     | 6008 | CLA  | C1C-C2C-C3C | -4.12 | 102.65      | 106.98   |
| 25  | T     | 6048 | BCR  | C33-C5-C6   | -4.12 | 119.99      | 124.48   |
| 22  | B     | 1020 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 22  | b     | 6019 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 22  | c     | 6026 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 22  | a     | 6006 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 22  | b     | 6020 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 25  | B     | 1048 | BCR  | C33-C5-C6   | -4.11 | 120.00      | 124.48   |
| 22  | b     | 6022 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 25  | B     | 1045 | BCR  | C38-C26-C25 | -4.11 | 120.00      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1014 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 22  | b     | 6018 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 22  | B     | 1010 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 22  | B     | 1016 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 22  | b     | 6024 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 22  | C     | 1027 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 25  | z     | 6053 | BCR  | C38-C26-C25 | -4.11 | 120.00      | 124.48   |
| 25  | C     | 1052 | BCR  | C33-C5-C6   | -4.11 | 120.00      | 124.48   |
| 22  | B     | 1022 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 25  | c     | 6054 | BCR  | C33-C5-C6   | -4.10 | 120.00      | 124.48   |
| 22  | C     | 1027 | CLA  | C3C-C4C-NC  | 4.10  | 115.69      | 110.43   |
| 22  | c     | 6035 | CLA  | C3C-C4C-NC  | 4.10  | 115.69      | 110.43   |
| 22  | A     | 1006 | CLA  | C1C-C2C-C3C | -4.10 | 102.67      | 106.98   |
| 22  | B     | 1024 | CLA  | C1C-C2C-C3C | -4.10 | 102.67      | 106.98   |
| 22  | c     | 6030 | CLA  | C1C-C2C-C3C | -4.10 | 102.67      | 106.98   |
| 25  | b     | 6047 | BCR  | C30-C25-C24 | 4.10  | 126.77      | 115.65   |
| 22  | c     | 6036 | CLA  | C1C-C2C-C3C | -4.10 | 102.67      | 106.98   |
| 22  | C     | 1033 | CLA  | C1C-C2C-C3C | -4.10 | 102.67      | 106.98   |
| 25  | D     | 1050 | BCR  | C33-C5-C6   | -4.10 | 120.01      | 124.48   |
| 22  | a     | 6003 | CLA  | C3C-C4C-NC  | 4.10  | 115.68      | 110.43   |
| 22  | b     | 6016 | CLA  | C3C-C4C-NC  | 4.10  | 115.68      | 110.43   |
| 22  | b     | 6020 | CLA  | C3B-C4B-NB  | 4.09  | 114.19      | 110.53   |
| 22  | H     | 1017 | CLA  | C1C-C2C-C3C | -4.09 | 102.67      | 106.98   |
| 25  | B     | 1048 | BCR  | C38-C26-C25 | -4.09 | 120.02      | 124.48   |
| 25  | b     | 6047 | BCR  | C33-C5-C6   | -4.09 | 120.02      | 124.48   |
| 22  | B     | 1010 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | b     | 6010 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | b     | 6015 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | b     | 6009 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 25  | B     | 1047 | BCR  | C30-C25-C24 | 4.09  | 126.75      | 115.65   |
| 22  | B     | 1023 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | b     | 6013 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | K     | 1034 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 25  | A     | 1044 | BCR  | C15-C14-C13 | -4.09 | 121.54      | 127.28   |
| 22  | B     | 1009 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | B     | 1016 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | b     | 6010 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | c     | 6027 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | B     | 1019 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 25  | z     | 6053 | BCR  | C33-C5-C6   | -4.09 | 120.02      | 124.48   |
| 22  | b     | 6020 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | c     | 6032 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1030 | CLA  | CHD-C4C-C3C | -4.09 | 118.81      | 124.77   |
| 22  | B     | 1013 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | c     | 6033 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 25  | A     | 1044 | BCR  | C33-C5-C6   | -4.09 | 120.02      | 124.48   |
| 25  | Z     | 1053 | BCR  | C33-C5-C6   | -4.09 | 120.02      | 124.48   |
| 22  | B     | 1013 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | c     | 6030 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 22  | h     | 6017 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 25  | C     | 1054 | BCR  | C33-C5-C6   | -4.09 | 120.03      | 124.48   |
| 22  | b     | 6016 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | c     | 6035 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | B     | 1015 | CLA  | C3C-C4C-NC  | 4.09  | 115.66      | 110.43   |
| 22  | C     | 1031 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 22  | c     | 6030 | CLA  | CHD-C4C-C3C | -4.09 | 118.82      | 124.77   |
| 22  | C     | 1025 | CLA  | C1C-C2C-C3C | -4.08 | 102.68      | 106.98   |
| 22  | b     | 6010 | CLA  | C3B-C4B-NB  | 4.08  | 114.18      | 110.53   |
| 25  | b     | 6047 | BCR  | C38-C26-C25 | -4.08 | 120.03      | 124.48   |
| 22  | C     | 1036 | CLA  | C1C-C2C-C3C | -4.08 | 102.69      | 106.98   |
| 22  | B     | 1020 | CLA  | C3B-C4B-NB  | 4.08  | 114.17      | 110.53   |
| 22  | C     | 1035 | CLA  | C3C-C4C-NC  | 4.08  | 115.66      | 110.43   |
| 22  | B     | 1015 | CLA  | C1C-C2C-C3C | -4.08 | 102.69      | 106.98   |
| 22  | C     | 1026 | CLA  | C1C-C2C-C3C | -4.08 | 102.69      | 106.98   |
| 25  | d     | 6050 | BCR  | C33-C5-C6   | -4.08 | 120.03      | 124.48   |
| 22  | D     | 1004 | CLA  | C1C-C2C-C3C | -4.08 | 102.69      | 106.98   |
| 22  | H     | 1017 | CLA  | C3C-C4C-NC  | 4.08  | 115.66      | 110.43   |
| 22  | c     | 6036 | CLA  | C3B-C4B-NB  | 4.08  | 114.17      | 110.53   |
| 22  | b     | 6020 | CLA  | C1D-ND-C4D  | -4.08 | 103.45      | 106.31   |
| 25  | B     | 1047 | BCR  | C38-C26-C25 | -4.08 | 120.03      | 124.48   |
| 22  | C     | 1029 | CLA  | C3C-C4C-NC  | 4.08  | 115.65      | 110.43   |
| 22  | B     | 1018 | CLA  | C1C-C2C-C3C | -4.08 | 102.69      | 106.98   |
| 22  | k     | 6034 | CLA  | C3C-C4C-NC  | 4.08  | 115.65      | 110.43   |
| 22  | b     | 6015 | CLA  | C3B-C4B-NB  | 4.07  | 114.17      | 110.53   |
| 22  | b     | 6022 | CLA  | C3C-C4C-NC  | 4.07  | 115.65      | 110.43   |
| 22  | B     | 1022 | CLA  | C3C-C4C-NC  | 4.07  | 115.65      | 110.43   |
| 22  | C     | 1032 | CLA  | C3C-C4C-NC  | 4.07  | 115.65      | 110.43   |
| 22  | b     | 6019 | CLA  | C3C-C4C-NC  | 4.07  | 115.65      | 110.43   |
| 22  | b     | 6009 | CLA  | C3B-C4B-NB  | 4.07  | 114.17      | 110.53   |
| 22  | c     | 6025 | CLA  | C3C-C4C-NC  | 4.07  | 115.64      | 110.43   |
| 22  | c     | 6036 | CLA  | C3C-C4C-NC  | 4.07  | 115.64      | 110.43   |
| 22  | h     | 6017 | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |
| 22  | C     | 1026 | CLA  | C3C-C4C-NC  | 4.07  | 115.64      | 110.43   |
| 22  | c     | 6029 | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1014 | CLA  | C3C-C4C-NC  | 4.07  | 115.64      | 110.43   |
| 22  | C     | 1029 | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |
| 22  | A     | 1003 | CLA  | C3C-C4C-NC  | 4.07  | 115.64      | 110.43   |
| 22  | d     | 6005 | CLA  | C3C-C4C-NC  | 4.07  | 115.64      | 110.43   |
| 22  | B     | 1023 | CLA  | C1D-ND-C4D  | -4.07 | 103.46      | 106.31   |
| 22  | c     | 6025 | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |
| 22  | B     | 1024 | CLA  | C3C-C4C-NC  | 4.06  | 115.64      | 110.43   |
| 22  | a     | 6007 | CLA  | C3C-C4C-NC  | 4.06  | 115.64      | 110.43   |
| 25  | B     | 1048 | BCR  | C30-C25-C24 | 4.06  | 126.67      | 115.65   |
| 22  | B     | 1009 | CLA  | C3B-C4B-NB  | 4.06  | 114.16      | 110.53   |
| 22  | D     | 1004 | CLA  | C3C-C4C-NC  | 4.06  | 115.64      | 110.43   |
| 25  | T     | 6048 | BCR  | C30-C25-C24 | 4.06  | 126.67      | 115.65   |
| 22  | C     | 1035 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 22  | B     | 1010 | CLA  | C3B-C4B-NB  | 4.06  | 114.16      | 110.53   |
| 22  | c     | 6028 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 22  | B     | 1020 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | b     | 6013 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | b     | 6014 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | B     | 1015 | CLA  | C3B-C4B-NB  | 4.06  | 114.16      | 110.53   |
| 25  | a     | 6044 | BCR  | C15-C14-C13 | -4.06 | 121.58      | 127.28   |
| 22  | c     | 6033 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | c     | 6028 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 25  | a     | 6044 | BCR  | C33-C5-C6   | -4.06 | 120.05      | 124.48   |
| 22  | C     | 1028 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 22  | a     | 6003 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 22  | c     | 6029 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | C     | 1025 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | D     | 1005 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | B     | 1019 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | d     | 6004 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 22  | A     | 1003 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 22  | C     | 1032 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 22  | C     | 1033 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 25  | A     | 1044 | BCR  | C30-C25-C24 | 4.06  | 126.65      | 115.65   |
| 22  | a     | 6006 | CLA  | C3C-C4C-NC  | 4.06  | 115.62      | 110.43   |
| 22  | b     | 6023 | CLA  | C3C-C4C-NC  | 4.05  | 115.62      | 110.43   |
| 25  | a     | 6044 | BCR  | C30-C25-C24 | 4.05  | 126.65      | 115.65   |
| 22  | c     | 6033 | CLA  | C3B-C4B-NB  | 4.05  | 114.15      | 110.53   |
| 28  | d     | 6062 | MGE  | O2G-C1B-C2B | 4.05  | 120.25      | 111.48   |
| 22  | B     | 1021 | CLA  | C3C-C4C-NC  | 4.05  | 115.62      | 110.43   |
| 22  | C     | 1035 | CLA  | C3B-C4B-NB  | 4.05  | 114.15      | 110.53   |
| 22  | H     | 1017 | CLA  | C3B-C4B-NB  | 4.05  | 114.14      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1036 | CLA  | C3C-C4C-NC  | 4.05  | 115.61      | 110.43   |
| 22  | b     | 6016 | CLA  | C3B-C4B-NB  | 4.05  | 114.14      | 110.53   |
| 29  | c     | 6056 | DGD  | O2G-C1B-C2B | 4.05  | 120.24      | 111.48   |
| 22  | c     | 6026 | CLA  | C3C-C4C-NC  | 4.05  | 115.61      | 110.43   |
| 22  | C     | 1037 | CLA  | C1C-C2C-C3C | -4.05 | 102.72      | 106.98   |
| 22  | b     | 6023 | CLA  | C1D-ND-C4D  | -4.05 | 103.47      | 106.31   |
| 22  | c     | 6027 | CLA  | C1D-ND-C4D  | -4.04 | 103.47      | 106.31   |
| 22  | A     | 1007 | CLA  | C3C-C4C-NC  | 4.04  | 115.61      | 110.43   |
| 22  | b     | 6021 | CLA  | C3C-C4C-NC  | 4.04  | 115.61      | 110.43   |
| 22  | b     | 6011 | CLA  | O2D-CGD-CBD | 4.04  | 118.30      | 111.23   |
| 22  | C     | 1028 | CLA  | C3C-C4C-NC  | 4.04  | 115.61      | 110.43   |
| 22  | c     | 6032 | CLA  | C1C-C2C-C3C | -4.04 | 102.73      | 106.98   |
| 22  | B     | 1013 | CLA  | C3B-C4B-NB  | 4.04  | 114.14      | 110.53   |
| 22  | b     | 6013 | CLA  | C3B-C4B-NB  | 4.04  | 114.14      | 110.53   |
| 22  | c     | 6037 | CLA  | C3C-C4C-NC  | 4.04  | 115.61      | 110.43   |
| 29  | C     | 1056 | DGD  | O2G-C1B-C2B | 4.04  | 120.22      | 111.48   |
| 22  | h     | 6017 | CLA  | C1D-ND-C4D  | -4.04 | 103.48      | 106.31   |
| 22  | C     | 1032 | CLA  | C3B-C4B-NB  | 4.04  | 114.14      | 110.53   |
| 22  | C     | 1037 | CLA  | C3C-C4C-NC  | 4.04  | 115.60      | 110.43   |
| 22  | B     | 1012 | CLA  | C3C-C4C-NC  | 4.04  | 115.60      | 110.43   |
| 22  | B     | 1011 | CLA  | C1C-C2C-C3C | -4.04 | 102.73      | 106.98   |
| 25  | T     | 6048 | BCR  | C38-C26-C25 | -4.04 | 120.08      | 124.48   |
| 22  | A     | 1006 | CLA  | C3C-C4C-NC  | 4.04  | 115.60      | 110.43   |
| 22  | C     | 1031 | CLA  | C3C-C4C-NC  | 4.04  | 115.60      | 110.43   |
| 22  | C     | 1026 | CLA  | C3B-C4B-NB  | 4.04  | 114.13      | 110.53   |
| 28  | D     | 1062 | MGE  | O2G-C1B-C2B | 4.04  | 120.21      | 111.48   |
| 22  | d     | 6004 | CLA  | C1C-C2C-C3C | -4.04 | 102.74      | 106.98   |
| 22  | B     | 1011 | CLA  | O2D-CGD-CBD | 4.04  | 118.28      | 111.23   |
| 22  | B     | 1023 | CLA  | C3C-C4C-NC  | 4.03  | 115.60      | 110.43   |
| 22  | c     | 6026 | CLA  | C3B-C4B-NB  | 4.03  | 114.13      | 110.53   |
| 22  | b     | 6021 | CLA  | C1D-ND-C4D  | -4.03 | 103.48      | 106.31   |
| 22  | c     | 6025 | CLA  | C1D-ND-C4D  | -4.03 | 103.48      | 106.31   |
| 22  | C     | 1030 | CLA  | C3B-C4B-NB  | 4.03  | 114.13      | 110.53   |
| 22  | c     | 6035 | CLA  | C3B-C4B-NB  | 4.03  | 114.13      | 110.53   |
| 29  | c     | 6057 | DGD  | O2G-C1B-C2B | 4.03  | 120.20      | 111.48   |
| 22  | b     | 6016 | CLA  | C1D-ND-C4D  | -4.03 | 103.48      | 106.31   |
| 22  | a     | 6007 | CLA  | C3B-C4B-NB  | 4.03  | 114.13      | 110.53   |
| 22  | B     | 1021 | CLA  | C3B-C4B-NB  | 4.03  | 114.13      | 110.53   |
| 22  | D     | 1004 | CLA  | C3B-C4B-NB  | 4.03  | 114.13      | 110.53   |
| 29  | C     | 1057 | DGD  | O2G-C1B-C2B | 4.03  | 120.19      | 111.48   |
| 22  | c     | 6037 | CLA  | C3B-C4B-NB  | 4.03  | 114.12      | 110.53   |
| 22  | B     | 1018 | CLA  | C3C-C4C-NC  | 4.03  | 115.59      | 110.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6012 | CLA  | C3C-C4C-NC  | 4.02  | 115.58      | 110.43   |
| 22  | B     | 1016 | CLA  | C3B-C4B-NB  | 4.02  | 114.12      | 110.53   |
| 28  | l     | 6061 | MGE  | O2G-C1B-C2B | 4.02  | 120.18      | 111.48   |
| 26  | a     | 6063 | LHG  | O7-C7-C8    | 4.02  | 120.18      | 111.48   |
| 28  | b     | 6060 | MGE  | O2G-C1B-C2B | 4.02  | 120.18      | 111.48   |
| 22  | A     | 1007 | CLA  | C3B-C4B-NB  | 4.02  | 114.12      | 110.53   |
| 22  | b     | 6018 | CLA  | C3B-C4B-NB  | 4.02  | 114.12      | 110.53   |
| 28  | B     | 1060 | MGE  | O2G-C1B-C2B | 4.02  | 120.17      | 111.48   |
| 22  | C     | 1033 | CLA  | C1D-ND-C4D  | -4.02 | 103.49      | 106.31   |
| 22  | c     | 6027 | CLA  | C3B-C4B-NB  | 4.02  | 114.11      | 110.53   |
| 22  | b     | 6024 | CLA  | C3C-C4C-NC  | 4.02  | 115.57      | 110.43   |
| 22  | b     | 6021 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | D     | 1008 | CLA  | C3C-C4C-NC  | 4.01  | 115.57      | 110.43   |
| 22  | C     | 1037 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | b     | 6019 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | a     | 6007 | CLA  | C1D-ND-C4D  | -4.01 | 103.50      | 106.31   |
| 28  | L     | 1061 | MGE  | O2G-C1B-C2B | 4.01  | 120.16      | 111.48   |
| 22  | A     | 1003 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | C     | 1031 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | k     | 6034 | CLA  | C1D-ND-C4D  | -4.01 | 103.50      | 106.31   |
| 22  | B     | 1018 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | h     | 6017 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | b     | 6012 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 22  | d     | 6008 | CLA  | C3C-C4C-NC  | 4.01  | 115.57      | 110.43   |
| 22  | B     | 1018 | CLA  | C1D-ND-C4D  | -4.01 | 103.50      | 106.31   |
| 22  | B     | 1021 | CLA  | C1D-ND-C4D  | -4.01 | 103.50      | 106.31   |
| 22  | c     | 6037 | CLA  | C1C-C2C-C3C | -4.01 | 102.77      | 106.98   |
| 29  | C     | 1055 | DGD  | O2G-C1B-C2B | 4.01  | 120.15      | 111.48   |
| 22  | B     | 1019 | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 26  | A     | 1063 | LHG  | O7-C7-C8    | 4.00  | 120.14      | 111.48   |
| 29  | B     | 1058 | DGD  | O2G-C1B-C2B | 4.00  | 120.14      | 111.48   |
| 22  | C     | 1036 | CLA  | C3B-C4B-NB  | 4.00  | 114.11      | 110.53   |
| 22  | a     | 6006 | CLA  | C3B-C4B-NB  | 4.00  | 114.11      | 110.53   |
| 29  | c     | 6055 | DGD  | O2G-C1B-C2B | 4.00  | 120.14      | 111.48   |
| 22  | c     | 6031 | CLA  | C3C-C4C-NC  | 4.00  | 115.55      | 110.43   |
| 22  | b     | 6011 | CLA  | C1C-C2C-C3C | -4.00 | 102.78      | 106.98   |
| 22  | B     | 1012 | CLA  | C3B-C4B-NB  | 4.00  | 114.10      | 110.53   |
| 22  | c     | 6028 | CLA  | C3B-C4B-NB  | 4.00  | 114.10      | 110.53   |
| 22  | c     | 6030 | CLA  | C3B-C4B-NB  | 4.00  | 114.10      | 110.53   |
| 29  | b     | 6058 | DGD  | O2G-C1B-C2B | 3.99  | 120.12      | 111.48   |
| 22  | C     | 1033 | CLA  | C3B-C4B-NB  | 3.99  | 114.10      | 110.53   |
| 22  | b     | 6023 | CLA  | C3B-C4B-NB  | 3.99  | 114.10      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6018 | CLA  | C3C-C4C-NC  | 3.99  | 115.55      | 110.43   |
| 22  | C     | 1027 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | a     | 6003 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | c     | 6032 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | B     | 1020 | CLA  | C1D-ND-C4D  | -3.99 | 103.51      | 106.31   |
| 22  | C     | 1025 | CLA  | C1D-ND-C4D  | -3.99 | 103.51      | 106.31   |
| 22  | b     | 6018 | CLA  | C1D-ND-C4D  | -3.99 | 103.51      | 106.31   |
| 22  | B     | 1014 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | B     | 1022 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | C     | 1028 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | b     | 6014 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | k     | 6034 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 22  | B     | 1015 | CLA  | C1D-ND-C4D  | -3.99 | 103.51      | 106.31   |
| 22  | H     | 1017 | CLA  | C1D-ND-C4D  | -3.99 | 103.51      | 106.31   |
| 22  | B     | 1014 | CLA  | C1D-ND-C4D  | -3.99 | 103.52      | 106.31   |
| 22  | c     | 6030 | CLA  | C1D-ND-C4D  | -3.99 | 103.52      | 106.31   |
| 22  | c     | 6031 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 28  | D     | 1059 | MGE  | O2G-C1B-C2B | 3.99  | 120.10      | 111.48   |
| 22  | b     | 6022 | CLA  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | B     | 1022 | CLA  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | b     | 6014 | CLA  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | B     | 1023 | CLA  | C3B-C4B-NB  | 3.98  | 114.09      | 110.53   |
| 22  | b     | 6012 | CLA  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | d     | 6004 | CLA  | C3B-C4B-NB  | 3.98  | 114.08      | 110.53   |
| 22  | a     | 6006 | CLA  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | c     | 6026 | CLA  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | b     | 6024 | CLA  | C3B-C4B-NB  | 3.98  | 114.08      | 110.53   |
| 22  | c     | 6029 | CLA  | C3B-C4B-NB  | 3.98  | 114.08      | 110.53   |
| 22  | c     | 6036 | CLA  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | b     | 6015 | CLA  | C1D-ND-C4D  | -3.97 | 103.52      | 106.31   |
| 22  | b     | 6011 | CLA  | CHD-C4C-C3C | -3.97 | 118.98      | 124.77   |
| 22  | C     | 1027 | CLA  | C1D-ND-C4D  | -3.97 | 103.52      | 106.31   |
| 28  | d     | 6059 | MGE  | O2G-C1B-C2B | 3.97  | 120.08      | 111.48   |
| 22  | C     | 1025 | CLA  | C3B-C4B-NB  | 3.97  | 114.08      | 110.53   |
| 22  | K     | 1034 | CLA  | C3B-C4B-NB  | 3.97  | 114.07      | 110.53   |
| 22  | B     | 1011 | CLA  | CHD-C4C-C3C | -3.97 | 118.99      | 124.77   |
| 22  | D     | 1005 | CLA  | C3B-C4B-NB  | 3.97  | 114.07      | 110.53   |
| 22  | A     | 1006 | CLA  | C3B-C4B-NB  | 3.97  | 114.07      | 110.53   |
| 22  | c     | 6025 | CLA  | C3B-C4B-NB  | 3.97  | 114.07      | 110.53   |
| 22  | A     | 1007 | CLA  | C1D-ND-C4D  | -3.96 | 103.53      | 106.31   |
| 22  | B     | 1024 | CLA  | C3B-C4B-NB  | 3.96  | 114.07      | 110.53   |
| 22  | C     | 1035 | CLA  | C1D-ND-C4D  | -3.96 | 103.53      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | K     | 1034 | CLA  | C1D-ND-C4D | -3.96 | 103.53      | 106.31   |
| 22  | d     | 6005 | CLA  | C3B-C4B-NB | 3.96  | 114.07      | 110.53   |
| 22  | d     | 6005 | CLA  | C1D-ND-C4D | -3.96 | 103.53      | 106.31   |
| 22  | A     | 1006 | CLA  | C1D-ND-C4D | -3.96 | 103.53      | 106.31   |
| 22  | C     | 1029 | CLA  | C3B-C4B-NB | 3.96  | 114.06      | 110.53   |
| 22  | A     | 1003 | CLA  | C1D-ND-C4D | -3.96 | 103.54      | 106.31   |
| 25  | T     | 6046 | BCR  | C7-C8-C9   | 3.96  | 132.09      | 126.23   |
| 22  | C     | 1030 | CLA  | C1D-ND-C4D | -3.95 | 103.54      | 106.31   |
| 22  | D     | 1005 | CLA  | C1D-ND-C4D | -3.95 | 103.54      | 106.31   |
| 22  | D     | 1004 | CLA  | C1D-ND-C4D | -3.95 | 103.54      | 106.31   |
| 22  | C     | 1026 | CLA  | C1D-ND-C4D | -3.95 | 103.54      | 106.31   |
| 22  | B     | 1012 | CLA  | C1D-ND-C4D | -3.95 | 103.54      | 106.31   |
| 22  | b     | 6011 | CLA  | C3B-C4B-NB | 3.95  | 114.05      | 110.53   |
| 22  | C     | 1036 | CLA  | C1D-ND-C4D | -3.94 | 103.55      | 106.31   |
| 22  | C     | 1037 | CLA  | C1D-ND-C4D | -3.94 | 103.55      | 106.31   |
| 22  | b     | 6022 | CLA  | C3B-C4B-NB | 3.94  | 114.05      | 110.53   |
| 25  | t     | 1046 | BCR  | C7-C8-C9   | 3.94  | 132.06      | 126.23   |
| 22  | c     | 6032 | CLA  | C1D-ND-C4D | -3.93 | 103.55      | 106.31   |
| 22  | c     | 6035 | CLA  | C1D-ND-C4D | -3.93 | 103.55      | 106.31   |
| 22  | B     | 1016 | CLA  | C1D-ND-C4D | -3.93 | 103.56      | 106.31   |
| 22  | c     | 6029 | CLA  | C1D-ND-C4D | -3.93 | 103.56      | 106.31   |
| 22  | c     | 6028 | CLA  | C1D-ND-C4D | -3.93 | 103.56      | 106.31   |
| 22  | C     | 1031 | CLA  | C1D-ND-C4D | -3.92 | 103.56      | 106.31   |
| 22  | B     | 1011 | CLA  | C3B-C4B-NB | 3.92  | 114.03      | 110.53   |
| 22  | b     | 6022 | CLA  | C3D-C4D-ND | 3.92  | 116.36      | 109.99   |
| 22  | a     | 6006 | CLA  | C3D-C4D-ND | 3.92  | 116.36      | 109.99   |
| 22  | C     | 1028 | CLA  | C1D-ND-C4D | -3.92 | 103.56      | 106.31   |
| 22  | B     | 1023 | CLA  | C3D-C4D-ND | 3.92  | 116.36      | 109.99   |
| 22  | C     | 1032 | CLA  | C1D-ND-C4D | -3.92 | 103.56      | 106.31   |
| 22  | c     | 6033 | CLA  | C1D-ND-C4D | -3.92 | 103.56      | 106.31   |
| 22  | B     | 1013 | CLA  | C1D-ND-C4D | -3.91 | 103.57      | 106.31   |
| 22  | d     | 6004 | CLA  | C1D-ND-C4D | -3.91 | 103.57      | 106.31   |
| 22  | B     | 1024 | CLA  | C1D-ND-C4D | -3.91 | 103.57      | 106.31   |
| 22  | B     | 1022 | CLA  | C3D-C4D-ND | 3.91  | 116.34      | 109.99   |
| 22  | b     | 6023 | CLA  | C3D-C4D-ND | 3.90  | 116.33      | 109.99   |
| 22  | B     | 1010 | CLA  | C1D-ND-C4D | -3.90 | 103.57      | 106.31   |
| 22  | c     | 6037 | CLA  | C1D-ND-C4D | -3.90 | 103.57      | 106.31   |
| 22  | h     | 6017 | CLA  | C3D-C4D-ND | 3.90  | 116.33      | 109.99   |
| 22  | C     | 1029 | CLA  | C1D-ND-C4D | -3.90 | 103.57      | 106.31   |
| 22  | C     | 1033 | CLA  | C3D-C4D-ND | 3.90  | 116.33      | 109.99   |
| 22  | k     | 6034 | CLA  | C3D-C4D-ND | 3.90  | 116.33      | 109.99   |
| 22  | b     | 6019 | CLA  | C1D-ND-C4D | -3.90 | 103.58      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6016 | CLA  | C3D-C4D-ND  | 3.90  | 116.33      | 109.99   |
| 22  | a     | 6003 | CLA  | C1D-ND-C4D  | -3.90 | 103.58      | 106.31   |
| 22  | c     | 6031 | CLA  | C1D-ND-C4D  | -3.90 | 103.58      | 106.31   |
| 25  | C     | 1052 | BCR  | C38-C26-C27 | 3.90  | 121.91      | 113.60   |
| 22  | B     | 1019 | CLA  | C1D-ND-C4D  | -3.90 | 103.58      | 106.31   |
| 22  | H     | 1017 | CLA  | C3D-C4D-ND  | 3.89  | 116.31      | 109.99   |
| 22  | b     | 6023 | CLA  | CHD-C4C-C3C | -3.89 | 119.10      | 124.77   |
| 22  | B     | 1015 | CLA  | C3D-C4D-ND  | 3.89  | 116.31      | 109.99   |
| 22  | b     | 6010 | CLA  | C1D-ND-C4D  | -3.89 | 103.58      | 106.31   |
| 22  | b     | 6021 | CLA  | C3D-C4D-ND  | 3.89  | 116.31      | 109.99   |
| 22  | c     | 6030 | CLA  | O2D-CGD-CBD | 3.89  | 118.03      | 111.23   |
| 22  | B     | 1013 | CLA  | C3D-C4D-ND  | 3.89  | 116.30      | 109.99   |
| 22  | C     | 1037 | CLA  | C3D-C4D-ND  | 3.89  | 116.30      | 109.99   |
| 22  | b     | 6015 | CLA  | C3D-C4D-ND  | 3.89  | 116.30      | 109.99   |
| 25  | k     | 6052 | BCR  | C38-C26-C27 | 3.89  | 121.88      | 113.60   |
| 22  | c     | 6026 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 22  | b     | 6013 | CLA  | C1D-ND-C4D  | -3.88 | 103.59      | 106.31   |
| 22  | C     | 1026 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 22  | B     | 1018 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 22  | A     | 1006 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 22  | d     | 6005 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 22  | c     | 6025 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 22  | B     | 1021 | CLA  | CHD-C4C-C3C | -3.88 | 119.12      | 124.77   |
| 22  | b     | 6014 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 22  | D     | 1005 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 22  | a     | 6007 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 22  | B     | 1021 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 22  | C     | 1025 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 22  | b     | 6018 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 22  | b     | 6012 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | c     | 6035 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | C     | 1036 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | c     | 6036 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | b     | 6021 | CLA  | CHD-C4C-C3C | -3.87 | 119.13      | 124.77   |
| 22  | D     | 1004 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | b     | 6013 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | c     | 6037 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | C     | 1035 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 22  | B     | 1023 | CLA  | CHD-C4C-C3C | -3.87 | 119.13      | 124.77   |
| 22  | C     | 1030 | CLA  | O2D-CGD-CBD | 3.87  | 117.99      | 111.23   |
| 22  | b     | 6020 | CLA  | C3D-C4D-ND  | 3.87  | 116.27      | 109.99   |
| 22  | B     | 1016 | CLA  | C3D-C4D-ND  | 3.87  | 116.27      | 109.99   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | K     | 1034 | CLA  | C3D-C4D-ND  | 3.87  | 116.27      | 109.99   |
| 22  | C     | 1029 | CLA  | CHD-C4C-C3C | -3.86 | 119.14      | 124.77   |
| 22  | c     | 6032 | CLA  | C3D-C4D-ND  | 3.86  | 116.27      | 109.99   |
| 22  | B     | 1009 | CLA  | CHD-C4C-C3C | -3.86 | 119.14      | 124.77   |
| 22  | A     | 1003 | CLA  | C3D-C4D-ND  | 3.86  | 116.27      | 109.99   |
| 22  | B     | 1020 | CLA  | C3D-C4D-ND  | 3.86  | 116.27      | 109.99   |
| 22  | C     | 1028 | CLA  | C3D-C4D-ND  | 3.86  | 116.26      | 109.99   |
| 22  | B     | 1014 | CLA  | C3D-C4D-ND  | 3.86  | 116.26      | 109.99   |
| 22  | c     | 6028 | CLA  | C3D-C4D-ND  | 3.86  | 116.26      | 109.99   |
| 22  | B     | 1013 | CLA  | CHD-C4C-C3C | -3.86 | 119.15      | 124.77   |
| 22  | c     | 6027 | CLA  | C3D-C4D-ND  | 3.86  | 116.26      | 109.99   |
| 22  | b     | 6019 | CLA  | C3D-C4D-ND  | 3.86  | 116.25      | 109.99   |
| 22  | B     | 1012 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 22  | b     | 6016 | CLA  | CHD-C4C-C3C | -3.85 | 119.15      | 124.77   |
| 22  | c     | 6033 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 22  | b     | 6009 | CLA  | CHD-C4C-C3C | -3.85 | 119.15      | 124.77   |
| 22  | A     | 1007 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 22  | b     | 6024 | CLA  | C1D-ND-C4D  | -3.85 | 103.61      | 106.31   |
| 22  | B     | 1024 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 22  | C     | 1032 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 22  | C     | 1037 | CLA  | CHD-C4C-C3C | -3.85 | 119.16      | 124.77   |
| 22  | B     | 1019 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 22  | C     | 1027 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 22  | b     | 6020 | CLA  | CHD-C4C-C3C | -3.85 | 119.16      | 124.77   |
| 22  | C     | 1031 | CLA  | C3D-C4D-ND  | 3.85  | 116.24      | 109.99   |
| 22  | C     | 1031 | CLA  | CHD-C4C-C3C | -3.85 | 119.17      | 124.77   |
| 25  | t     | 1046 | BCR  | C1-C6-C5    | -3.85 | 117.38      | 122.64   |
| 22  | b     | 6022 | CLA  | CHD-C4C-C3C | -3.85 | 119.17      | 124.77   |
| 22  | b     | 6015 | CLA  | CHD-C4C-C3C | -3.85 | 119.17      | 124.77   |
| 22  | c     | 6032 | CLA  | CHD-C4C-C3C | -3.84 | 119.17      | 124.77   |
| 22  | d     | 6005 | CLA  | CHD-C4C-C3C | -3.84 | 119.17      | 124.77   |
| 22  | d     | 6004 | CLA  | C3D-C4D-ND  | 3.84  | 116.23      | 109.99   |
| 22  | b     | 6011 | CLA  | C1D-ND-C4D  | -3.84 | 103.62      | 106.31   |
| 22  | B     | 1014 | CLA  | CHD-C4C-C3C | -3.84 | 119.17      | 124.77   |
| 22  | C     | 1027 | CLA  | CHD-C4C-C3C | -3.84 | 119.17      | 124.77   |
| 22  | c     | 6029 | CLA  | CHD-C4C-C3C | -3.84 | 119.17      | 124.77   |
| 22  | b     | 6013 | CLA  | CHD-C4C-C3C | -3.84 | 119.17      | 124.77   |
| 22  | C     | 1032 | CLA  | CHD-C4C-C3C | -3.84 | 119.18      | 124.77   |
| 22  | B     | 1022 | CLA  | CHD-C4C-C3C | -3.84 | 119.18      | 124.77   |
| 22  | c     | 6025 | CLA  | CHD-C4C-C3C | -3.84 | 119.18      | 124.77   |
| 22  | c     | 6031 | CLA  | CHD-C4C-C3C | -3.84 | 119.18      | 124.77   |
| 22  | c     | 6029 | CLA  | C3D-C4D-ND  | 3.84  | 116.23      | 109.99   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6014 | CLA  | CHD-C4C-C3C | -3.84 | 119.18      | 124.77   |
| 22  | B     | 1024 | CLA  | CHD-C4C-C3C | -3.84 | 119.18      | 124.77   |
| 22  | B     | 1016 | CLA  | CHD-C4C-C3C | -3.83 | 119.18      | 124.77   |
| 22  | a     | 6003 | CLA  | C3D-C4D-ND  | 3.83  | 116.22      | 109.99   |
| 22  | c     | 6035 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | b     | 6010 | CLA  | C3D-C4D-ND  | 3.83  | 116.22      | 109.99   |
| 22  | d     | 6008 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | C     | 1028 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | B     | 1020 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | D     | 1004 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | c     | 6037 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | b     | 6018 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | A     | 1003 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | a     | 6007 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | B     | 1018 | CLA  | CHD-C4C-C3C | -3.83 | 119.19      | 124.77   |
| 22  | b     | 6024 | CLA  | C3D-C4D-ND  | 3.82  | 116.20      | 109.99   |
| 22  | a     | 6003 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | b     | 6010 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | h     | 6017 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | c     | 6031 | CLA  | C3D-C4D-ND  | 3.82  | 116.20      | 109.99   |
| 22  | H     | 1017 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | K     | 1034 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | C     | 1029 | CLA  | C3D-C4D-ND  | 3.82  | 116.20      | 109.99   |
| 22  | A     | 1007 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | B     | 1010 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | D     | 1005 | CLA  | CHD-C4C-C3C | -3.82 | 119.20      | 124.77   |
| 22  | C     | 1025 | CLA  | CHD-C4C-C3C | -3.82 | 119.21      | 124.77   |
| 22  | B     | 1010 | CLA  | C3D-C4D-ND  | 3.82  | 116.19      | 109.99   |
| 22  | c     | 6027 | CLA  | CHD-C4C-C3C | -3.82 | 119.21      | 124.77   |
| 22  | c     | 6028 | CLA  | CHD-C4C-C3C | -3.81 | 119.21      | 124.77   |
| 22  | B     | 1015 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | C     | 1035 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | k     | 6034 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | a     | 6006 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | c     | 6030 | CLA  | C3D-C4D-ND  | 3.81  | 116.18      | 109.99   |
| 22  | d     | 6004 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | C     | 1036 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 25  | T     | 6046 | BCR  | C1-C6-C5    | -3.81 | 117.43      | 122.64   |
| 22  | C     | 1026 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | C     | 1033 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | B     | 1012 | CLA  | CHD-C4C-C3C | -3.81 | 119.22      | 124.77   |
| 22  | A     | 1006 | CLA  | CHD-C4C-C3C | -3.80 | 119.23      | 124.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1030 | CLA  | C3D-C4D-ND  | 3.80  | 116.17      | 109.99   |
| 22  | b     | 6009 | CLA  | C1D-ND-C4D  | -3.80 | 103.65      | 106.31   |
| 22  | D     | 1008 | CLA  | C3D-C4D-ND  | 3.80  | 116.16      | 109.99   |
| 22  | D     | 1008 | CLA  | CHD-C4C-C3C | -3.80 | 119.24      | 124.77   |
| 22  | b     | 6024 | CLA  | CHD-C4C-C3C | -3.80 | 119.24      | 124.77   |
| 22  | c     | 6026 | CLA  | CHD-C4C-C3C | -3.79 | 119.24      | 124.77   |
| 22  | c     | 6036 | CLA  | CHD-C4C-C3C | -3.79 | 119.24      | 124.77   |
| 22  | d     | 6008 | CLA  | C1D-ND-C4D  | -3.79 | 103.65      | 106.31   |
| 22  | b     | 6019 | CLA  | CHD-C4C-C3C | -3.79 | 119.25      | 124.77   |
| 22  | d     | 6008 | CLA  | C3D-C4D-ND  | 3.79  | 116.15      | 109.99   |
| 22  | c     | 6033 | CLA  | CHD-C4C-C3C | -3.78 | 119.26      | 124.77   |
| 22  | b     | 6012 | CLA  | CHD-C4C-C3C | -3.78 | 119.26      | 124.77   |
| 22  | B     | 1011 | CLA  | C1D-ND-C4D  | -3.78 | 103.66      | 106.31   |
| 22  | B     | 1019 | CLA  | CHD-C4C-C3C | -3.78 | 119.27      | 124.77   |
| 25  | a     | 6044 | BCR  | C38-C26-C25 | -3.76 | 120.38      | 124.48   |
| 22  | B     | 1009 | CLA  | C1D-ND-C4D  | -3.76 | 103.67      | 106.31   |
| 22  | b     | 6011 | CLA  | C3D-C4D-ND  | 3.76  | 116.10      | 109.99   |
| 22  | D     | 1008 | CLA  | C1D-ND-C4D  | -3.76 | 103.68      | 106.31   |
| 22  | b     | 6009 | CLA  | C3D-C4D-ND  | 3.75  | 116.08      | 109.99   |
| 22  | B     | 1009 | CLA  | C3D-C4D-ND  | 3.74  | 116.07      | 109.99   |
| 22  | B     | 1011 | CLA  | C3D-C4D-ND  | 3.74  | 116.07      | 109.99   |
| 25  | A     | 1044 | BCR  | C38-C26-C25 | -3.74 | 120.41      | 124.48   |
| 22  | D     | 1008 | CLA  | O2D-CGD-CBD | 3.70  | 117.69      | 111.23   |
| 24  | a     | 6043 | PQ9  | C11-C12-C13 | -3.69 | 120.47      | 126.83   |
| 22  | d     | 6008 | CLA  | O2D-CGD-CBD | 3.68  | 117.67      | 111.23   |
| 24  | A     | 1043 | PQ9  | C11-C12-C13 | -3.68 | 120.48      | 126.83   |
| 24  | d     | 6042 | PQ9  | C11-C12-C13 | -3.67 | 120.50      | 126.83   |
| 24  | D     | 1042 | PQ9  | C11-C12-C13 | -3.67 | 120.51      | 126.83   |
| 23  | D     | 1039 | PHO  | OBD-CAD-CBD | -3.64 | 120.47      | 125.82   |
| 25  | a     | 6044 | BCR  | C37-C22-C23 | 3.63  | 123.63      | 118.09   |
| 25  | A     | 1044 | BCR  | C37-C22-C23 | 3.63  | 123.63      | 118.09   |
| 23  | d     | 6039 | PHO  | OBD-CAD-CBD | -3.62 | 120.51      | 125.82   |
| 23  | a     | 6038 | PHO  | OBD-CAD-CBD | -3.62 | 120.52      | 125.82   |
| 23  | A     | 1038 | PHO  | OBD-CAD-CBD | -3.60 | 120.54      | 125.82   |
| 25  | T     | 6046 | BCR  | C38-C26-C25 | -3.57 | 120.59      | 124.48   |
| 25  | t     | 1046 | BCR  | C38-C26-C25 | -3.57 | 120.59      | 124.48   |
| 22  | b     | 6023 | CLA  | C2A-C1A-CHA | -3.55 | 117.70      | 123.87   |
| 22  | B     | 1023 | CLA  | C2A-C1A-CHA | -3.55 | 117.71      | 123.87   |
| 22  | b     | 6022 | CLA  | C2A-C1A-CHA | -3.54 | 117.72      | 123.87   |
| 22  | d     | 6008 | CLA  | C2A-C1A-CHA | -3.54 | 117.72      | 123.87   |
| 22  | b     | 6014 | CLA  | C2A-C1A-CHA | -3.54 | 117.73      | 123.87   |
| 22  | b     | 6016 | CLA  | C2A-C1A-CHA | -3.54 | 117.73      | 123.87   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1014 | CLA  | C2A-C1A-CHA | -3.53 | 117.73      | 123.87   |
| 22  | c     | 6025 | CLA  | C2A-C1A-CHA | -3.53 | 117.73      | 123.87   |
| 22  | D     | 1008 | CLA  | C2A-C1A-CHA | -3.53 | 117.74      | 123.87   |
| 22  | C     | 1037 | CLA  | C2A-C1A-CHA | -3.53 | 117.74      | 123.87   |
| 22  | c     | 6037 | CLA  | C2A-C1A-CHA | -3.53 | 117.74      | 123.87   |
| 22  | a     | 6006 | CLA  | C2A-C1A-CHA | -3.53 | 117.75      | 123.87   |
| 22  | C     | 1025 | CLA  | C2A-C1A-CHA | -3.52 | 117.75      | 123.87   |
| 22  | b     | 6013 | CLA  | C2A-C1A-CHA | -3.52 | 117.75      | 123.87   |
| 22  | c     | 6035 | CLA  | C2A-C1A-CHA | -3.52 | 117.75      | 123.87   |
| 22  | b     | 6022 | CLA  | C1-C2-C3    | -3.52 | 120.43      | 126.20   |
| 22  | k     | 6034 | CLA  | C2A-C1A-CHA | -3.52 | 117.76      | 123.87   |
| 22  | c     | 6028 | CLA  | C1-C2-C3    | -3.52 | 120.43      | 126.20   |
| 22  | c     | 6033 | CLA  | C2A-C1A-CHA | -3.52 | 117.76      | 123.87   |
| 22  | a     | 6003 | CLA  | C1-C2-C3    | -3.52 | 120.43      | 126.20   |
| 22  | d     | 6005 | CLA  | C2A-C1A-CHA | -3.52 | 117.76      | 123.87   |
| 22  | D     | 1005 | CLA  | C2A-C1A-CHA | -3.52 | 117.76      | 123.87   |
| 22  | A     | 1006 | CLA  | C2A-C1A-CHA | -3.52 | 117.76      | 123.87   |
| 22  | B     | 1022 | CLA  | C2A-C1A-CHA | -3.52 | 117.77      | 123.87   |
| 22  | C     | 1033 | CLA  | C2A-C1A-CHA | -3.51 | 117.77      | 123.87   |
| 22  | a     | 6007 | CLA  | C2A-C1A-CHA | -3.51 | 117.77      | 123.87   |
| 22  | b     | 6019 | CLA  | C2A-C1A-CHA | -3.51 | 117.77      | 123.87   |
| 22  | c     | 6037 | CLA  | C1-C2-C3    | -3.51 | 120.44      | 126.20   |
| 22  | B     | 1019 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | B     | 1009 | CLA  | C1-C2-C3    | -3.51 | 120.45      | 126.20   |
| 22  | H     | 1017 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | A     | 1003 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | B     | 1015 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | B     | 1021 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | C     | 1031 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | b     | 6015 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | c     | 6032 | CLA  | C1-C2-C3    | -3.51 | 120.45      | 126.20   |
| 22  | B     | 1013 | CLA  | C2A-C1A-CHA | -3.51 | 117.78      | 123.87   |
| 22  | b     | 6009 | CLA  | C1-C2-C3    | -3.50 | 120.45      | 126.20   |
| 22  | d     | 6004 | CLA  | C1-C2-C3    | -3.50 | 120.46      | 126.20   |
| 22  | A     | 1007 | CLA  | C2A-C1A-CHA | -3.50 | 117.79      | 123.87   |
| 22  | D     | 1004 | CLA  | C2A-C1A-CHA | -3.50 | 117.79      | 123.87   |
| 22  | C     | 1027 | CLA  | C2A-C1A-CHA | -3.50 | 117.79      | 123.87   |
| 22  | C     | 1036 | CLA  | C2A-C1A-CHA | -3.50 | 117.79      | 123.87   |
| 22  | K     | 1034 | CLA  | C2A-C1A-CHA | -3.50 | 117.79      | 123.87   |
| 22  | B     | 1022 | CLA  | C1-C2-C3    | -3.50 | 120.46      | 126.20   |
| 22  | c     | 6027 | CLA  | C1-C2-C3    | -3.50 | 120.46      | 126.20   |
| 22  | c     | 6036 | CLA  | C2A-C1A-CHA | -3.50 | 117.79      | 123.87   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1028 | CLA  | C2A-C1A-CHA | -3.50 | 117.80      | 123.87   |
| 22  | C     | 1028 | CLA  | C1-C2-C3    | -3.50 | 120.47      | 126.20   |
| 22  | d     | 6004 | CLA  | C2A-C1A-CHA | -3.50 | 117.80      | 123.87   |
| 22  | C     | 1033 | CLA  | C1-C2-C3    | -3.50 | 120.47      | 126.20   |
| 22  | C     | 1035 | CLA  | C2A-C1A-CHA | -3.50 | 117.80      | 123.87   |
| 22  | B     | 1016 | CLA  | C2A-C1A-CHA | -3.50 | 117.80      | 123.87   |
| 22  | B     | 1020 | CLA  | C2A-C1A-CHA | -3.50 | 117.80      | 123.87   |
| 22  | C     | 1032 | CLA  | C1-C2-C3    | -3.49 | 120.47      | 126.20   |
| 22  | B     | 1012 | CLA  | C2A-C1A-CHA | -3.49 | 117.80      | 123.87   |
| 22  | c     | 6031 | CLA  | C1-C2-C3    | -3.49 | 120.47      | 126.20   |
| 22  | c     | 6027 | CLA  | C2A-C1A-CHA | -3.49 | 117.80      | 123.87   |
| 22  | c     | 6032 | CLA  | C2A-C1A-CHA | -3.49 | 117.80      | 123.87   |
| 22  | B     | 1018 | CLA  | C2A-C1A-CHA | -3.49 | 117.80      | 123.87   |
| 22  | B     | 1024 | CLA  | C2A-C1A-CHA | -3.49 | 117.81      | 123.87   |
| 22  | C     | 1032 | CLA  | C2A-C1A-CHA | -3.49 | 117.81      | 123.87   |
| 22  | b     | 6024 | CLA  | C2A-C1A-CHA | -3.49 | 117.81      | 123.87   |
| 22  | c     | 6031 | CLA  | C2A-C1A-CHA | -3.49 | 117.81      | 123.87   |
| 22  | A     | 1003 | CLA  | C1-C2-C3    | -3.49 | 120.48      | 126.20   |
| 22  | b     | 6021 | CLA  | C2A-C1A-CHA | -3.49 | 117.81      | 123.87   |
| 22  | b     | 6024 | CLA  | C1-C2-C3    | -3.49 | 120.48      | 126.20   |
| 22  | c     | 6028 | CLA  | C2A-C1A-CHA | -3.49 | 117.81      | 123.87   |
| 22  | B     | 1016 | CLA  | C1-C2-C3    | -3.49 | 120.48      | 126.20   |
| 22  | c     | 6035 | CLA  | C1-C2-C3    | -3.49 | 120.48      | 126.20   |
| 22  | D     | 1005 | CLA  | C1-C2-C3    | -3.49 | 120.48      | 126.20   |
| 22  | b     | 6012 | CLA  | C2A-C1A-CHA | -3.49 | 117.82      | 123.87   |
| 22  | h     | 6017 | CLA  | C2A-C1A-CHA | -3.49 | 117.82      | 123.87   |
| 22  | B     | 1014 | CLA  | C1-C2-C3    | -3.49 | 120.49      | 126.20   |
| 22  | C     | 1036 | CLA  | C1-C2-C3    | -3.49 | 120.49      | 126.20   |
| 22  | C     | 1037 | CLA  | C1-C2-C3    | -3.49 | 120.49      | 126.20   |
| 22  | b     | 6014 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | b     | 6015 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | a     | 6003 | CLA  | C2A-C1A-CHA | -3.48 | 117.82      | 123.87   |
| 22  | C     | 1031 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | H     | 1017 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | K     | 1034 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | C     | 1026 | CLA  | C2A-C1A-CHA | -3.48 | 117.82      | 123.87   |
| 22  | c     | 6026 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | A     | 1006 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | C     | 1035 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | a     | 6006 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | a     | 6007 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | d     | 6005 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1019 | CLA  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 23  | D     | 1039 | PHO  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 22  | A     | 1007 | CLA  | C1-C2-C3    | -3.48 | 120.50      | 126.20   |
| 22  | C     | 1026 | CLA  | C1-C2-C3    | -3.48 | 120.50      | 126.20   |
| 22  | B     | 1012 | CLA  | C1-C2-C3    | -3.48 | 120.50      | 126.20   |
| 22  | h     | 6017 | CLA  | C1-C2-C3    | -3.48 | 120.50      | 126.20   |
| 22  | k     | 6034 | CLA  | C1-C2-C3    | -3.48 | 120.50      | 126.20   |
| 22  | B     | 1015 | CLA  | C1-C2-C3    | -3.48 | 120.50      | 126.20   |
| 22  | b     | 6018 | CLA  | C2A-C1A-CHA | -3.47 | 117.84      | 123.87   |
| 22  | C     | 1027 | CLA  | C1-C2-C3    | -3.47 | 120.50      | 126.20   |
| 22  | b     | 6018 | CLA  | C1-C2-C3    | -3.47 | 120.50      | 126.20   |
| 22  | c     | 6036 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | b     | 6016 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | B     | 1013 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | c     | 6033 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | D     | 1004 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | c     | 6025 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | B     | 1020 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | B     | 1018 | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 22  | b     | 6020 | CLA  | C2A-C1A-CHA | -3.47 | 117.85      | 123.87   |
| 22  | b     | 6012 | CLA  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 22  | c     | 6030 | CLA  | C2A-C1A-CHA | -3.47 | 117.85      | 123.87   |
| 22  | B     | 1024 | CLA  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 22  | b     | 6019 | CLA  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 23  | A     | 1038 | PHO  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 22  | b     | 6010 | CLA  | C2A-C1A-CHA | -3.47 | 117.85      | 123.87   |
| 22  | C     | 1025 | CLA  | C1-C2-C3    | -3.46 | 120.52      | 126.20   |
| 23  | d     | 6039 | PHO  | C1-C2-C3    | -3.46 | 120.52      | 126.20   |
| 22  | c     | 6026 | CLA  | C2A-C1A-CHA | -3.46 | 117.86      | 123.87   |
| 22  | B     | 1010 | CLA  | C2A-C1A-CHA | -3.46 | 117.86      | 123.87   |
| 23  | a     | 6038 | PHO  | C1-C2-C3    | -3.46 | 120.53      | 126.20   |
| 22  | b     | 6013 | CLA  | C1-C2-C3    | -3.46 | 120.54      | 126.20   |
| 22  | B     | 1011 | CLA  | C2A-C1A-CHA | -3.45 | 117.87      | 123.87   |
| 22  | b     | 6011 | CLA  | C2A-C1A-CHA | -3.45 | 117.88      | 123.87   |
| 22  | C     | 1030 | CLA  | C2A-C1A-CHA | -3.44 | 117.89      | 123.87   |
| 22  | b     | 6020 | CLA  | C1-C2-C3    | -3.44 | 120.56      | 126.20   |
| 22  | c     | 6029 | CLA  | C2A-C1A-CHA | -3.44 | 117.90      | 123.87   |
| 22  | C     | 1029 | CLA  | C2A-C1A-CHA | -3.43 | 117.91      | 123.87   |
| 22  | b     | 6010 | CLA  | C1-C2-C3    | -3.40 | 120.63      | 126.20   |
| 22  | B     | 1009 | CLA  | C2A-C1A-CHA | -3.39 | 117.98      | 123.87   |
| 22  | b     | 6009 | CLA  | C2A-C1A-CHA | -3.39 | 117.98      | 123.87   |
| 25  | t     | 1046 | BCR  | C33-C5-C6   | -3.38 | 120.79      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | T     | 6046 | BCR  | C33-C5-C4   | 3.37  | 120.79      | 113.60   |
| 22  | B     | 1010 | CLA  | C1-C2-C3    | -3.37 | 120.67      | 126.20   |
| 25  | T     | 6046 | BCR  | C33-C5-C6   | -3.36 | 120.82      | 124.48   |
| 22  | D     | 1008 | CLA  | C1-C2-C3    | -3.36 | 120.70      | 126.20   |
| 25  | t     | 1046 | BCR  | C33-C5-C4   | 3.36  | 120.75      | 113.60   |
| 22  | c     | 6029 | CLA  | C1-C2-C3    | -3.35 | 120.71      | 126.20   |
| 22  | C     | 1029 | CLA  | C1-C2-C3    | -3.33 | 120.73      | 126.20   |
| 24  | d     | 6042 | PQ9  | C11-C2-C1   | 3.33  | 119.66      | 116.91   |
| 22  | d     | 6008 | CLA  | C1-C2-C3    | -3.33 | 120.74      | 126.20   |
| 25  | k     | 6052 | BCR  | C37-C22-C23 | 3.32  | 123.16      | 118.09   |
| 25  | C     | 1052 | BCR  | C37-C22-C23 | 3.30  | 123.13      | 118.09   |
| 22  | b     | 6021 | CLA  | C1-C2-C3    | -3.29 | 120.81      | 126.20   |
| 24  | D     | 1042 | PQ9  | C11-C2-C1   | 3.28  | 119.61      | 116.91   |
| 24  | a     | 6043 | PQ9  | C11-C2-C1   | 3.28  | 119.61      | 116.91   |
| 24  | A     | 1043 | PQ9  | C11-C2-C1   | 3.28  | 119.61      | 116.91   |
| 22  | B     | 1021 | CLA  | C1-C2-C3    | -3.28 | 120.83      | 126.20   |
| 22  | B     | 1023 | CLA  | C1-C2-C3    | -3.27 | 120.83      | 126.20   |
| 22  | b     | 6023 | CLA  | C1-C2-C3    | -3.26 | 120.86      | 126.20   |
| 22  | B     | 1011 | CLA  | O2D-CGD-O1D | -3.26 | 117.50      | 123.85   |
| 22  | b     | 6011 | CLA  | O2D-CGD-O1D | -3.26 | 117.50      | 123.85   |
| 24  | d     | 6042 | PQ9  | C11-C2-C3   | -3.21 | 119.61      | 123.39   |
| 24  | a     | 6043 | PQ9  | C11-C2-C3   | -3.20 | 119.61      | 123.39   |
| 24  | A     | 1043 | PQ9  | C11-C2-C3   | -3.19 | 119.62      | 123.39   |
| 25  | T     | 6046 | BCR  | C4-C5-C6    | -3.19 | 118.39      | 122.70   |
| 22  | c     | 6030 | CLA  | C1-C2-C3    | -3.19 | 120.97      | 126.20   |
| 24  | D     | 1042 | PQ9  | C11-C2-C3   | -3.19 | 119.63      | 123.39   |
| 22  | C     | 1030 | CLA  | C1-C2-C3    | -3.18 | 120.99      | 126.20   |
| 22  | D     | 1008 | CLA  | CAC-C3C-C4C | 3.17  | 128.92      | 124.79   |
| 22  | d     | 6008 | CLA  | CAC-C3C-C4C | 3.16  | 128.90      | 124.79   |
| 25  | t     | 1046 | BCR  | C4-C5-C6    | -3.15 | 118.45      | 122.70   |
| 25  | B     | 1047 | BCR  | C37-C22-C21 | -3.14 | 117.72      | 122.82   |
| 24  | d     | 6042 | PQ9  | C26-C27-C28 | -3.14 | 120.44      | 127.62   |
| 24  | d     | 6042 | PQ9  | C16-C17-C18 | -3.13 | 120.45      | 127.62   |
| 24  | d     | 6042 | PQ9  | C31-C32-C33 | -3.13 | 120.46      | 127.62   |
| 22  | d     | 6008 | CLA  | O2D-CGD-O1D | -3.13 | 117.75      | 123.85   |
| 25  | b     | 6047 | BCR  | C37-C22-C21 | -3.13 | 117.75      | 122.82   |
| 22  | b     | 6010 | CLA  | CMB-C2B-C1B | 3.13  | 130.18      | 125.42   |
| 24  | D     | 1042 | PQ9  | C31-C32-C33 | -3.13 | 120.47      | 127.62   |
| 24  | d     | 6042 | PQ9  | C36-C37-C38 | -3.13 | 120.47      | 127.62   |
| 22  | D     | 1008 | CLA  | O2D-CGD-O1D | -3.13 | 117.76      | 123.85   |
| 24  | D     | 1042 | PQ9  | C26-C27-C28 | -3.12 | 120.47      | 127.62   |
| 24  | d     | 6042 | PQ9  | C21-C22-C23 | -3.12 | 120.48      | 127.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | D     | 1042 | PQ9  | C16-C17-C18 | -3.12 | 120.49      | 127.62   |
| 24  | a     | 6043 | PQ9  | C21-C22-C23 | -3.12 | 120.49      | 127.62   |
| 24  | A     | 1043 | PQ9  | C31-C32-C33 | -3.12 | 120.49      | 127.62   |
| 24  | D     | 1042 | PQ9  | C21-C22-C23 | -3.11 | 120.50      | 127.62   |
| 25  | B     | 1048 | BCR  | C37-C22-C21 | -3.11 | 117.77      | 122.82   |
| 24  | a     | 6043 | PQ9  | C31-C32-C33 | -3.11 | 120.50      | 127.62   |
| 22  | B     | 1010 | CLA  | CMB-C2B-C1B | 3.11  | 130.16      | 125.42   |
| 24  | A     | 1043 | PQ9  | C21-C22-C23 | -3.11 | 120.50      | 127.62   |
| 24  | D     | 1042 | PQ9  | C36-C37-C38 | -3.11 | 120.50      | 127.62   |
| 25  | T     | 6048 | BCR  | C37-C22-C21 | -3.11 | 117.78      | 122.82   |
| 24  | A     | 1043 | PQ9  | C26-C27-C28 | -3.11 | 120.52      | 127.62   |
| 24  | a     | 6043 | PQ9  | C26-C27-C28 | -3.10 | 120.53      | 127.62   |
| 24  | a     | 6043 | PQ9  | C16-C17-C18 | -3.10 | 120.53      | 127.62   |
| 24  | A     | 1043 | PQ9  | C16-C17-C18 | -3.09 | 120.54      | 127.62   |
| 22  | b     | 6011 | CLA  | C1-C2-C3    | -3.09 | 121.13      | 126.20   |
| 24  | a     | 6043 | PQ9  | C36-C37-C38 | -3.09 | 120.55      | 127.62   |
| 24  | A     | 1043 | PQ9  | C36-C37-C38 | -3.09 | 120.55      | 127.62   |
| 22  | B     | 1011 | CLA  | C1-C2-C3    | -3.09 | 121.14      | 126.20   |
| 25  | A     | 1044 | BCR  | C33-C5-C4   | 3.07  | 120.13      | 113.60   |
| 22  | d     | 6008 | CLA  | CMB-C2B-C1B | 3.07  | 130.09      | 125.42   |
| 25  | a     | 6044 | BCR  | C33-C5-C4   | 3.06  | 120.12      | 113.60   |
| 22  | b     | 6011 | CLA  | CMB-C2B-C1B | 3.05  | 130.07      | 125.42   |
| 22  | D     | 1008 | CLA  | CMB-C2B-C1B | 3.05  | 130.06      | 125.42   |
| 22  | B     | 1011 | CLA  | CMB-C2B-C1B | 3.04  | 130.05      | 125.42   |
| 25  | B     | 1048 | BCR  | C38-C26-C27 | 3.04  | 120.08      | 113.60   |
| 22  | b     | 6011 | CLA  | O1D-CGD-CBD | -3.04 | 118.53      | 124.52   |
| 25  | T     | 6048 | BCR  | C38-C26-C27 | 3.04  | 120.07      | 113.60   |
| 22  | B     | 1011 | CLA  | O1D-CGD-CBD | -3.03 | 118.55      | 124.52   |
| 22  | C     | 1029 | CLA  | CAC-C3C-C4C | 3.03  | 128.73      | 124.79   |
| 25  | c     | 6054 | BCR  | C33-C5-C4   | 3.03  | 120.05      | 113.60   |
| 25  | B     | 1048 | BCR  | C33-C5-C4   | 3.02  | 120.04      | 113.60   |
| 25  | z     | 6053 | BCR  | C38-C26-C27 | 3.02  | 120.04      | 113.60   |
| 25  | d     | 6050 | BCR  | C38-C26-C27 | 3.02  | 120.04      | 113.60   |
| 22  | c     | 6029 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 25  | b     | 6047 | BCR  | C38-C26-C27 | 3.02  | 120.04      | 113.60   |
| 25  | T     | 6048 | BCR  | C33-C5-C4   | 3.02  | 120.04      | 113.60   |
| 25  | D     | 1050 | BCR  | C38-C26-C27 | 3.02  | 120.03      | 113.60   |
| 22  | B     | 1010 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 25  | B     | 1045 | BCR  | C33-C5-C4   | 3.02  | 120.03      | 113.60   |
| 25  | Z     | 1053 | BCR  | C33-C5-C4   | 3.02  | 120.03      | 113.60   |
| 22  | b     | 6010 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 25  | b     | 6047 | BCR  | C33-C5-C4   | 3.02  | 120.03      | 113.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | C     | 1054 | BCR  | C33-C5-C4   | 3.01  | 120.02      | 113.60   |
| 25  | B     | 1047 | BCR  | C38-C26-C27 | 3.01  | 120.02      | 113.60   |
| 25  | z     | 6053 | BCR  | C33-C5-C4   | 3.01  | 120.02      | 113.60   |
| 25  | b     | 6045 | BCR  | C33-C5-C4   | 3.01  | 120.02      | 113.60   |
| 25  | k     | 6051 | BCR  | C33-C5-C4   | 3.01  | 120.02      | 113.60   |
| 25  | B     | 1047 | BCR  | C33-C5-C4   | 3.01  | 120.02      | 113.60   |
| 25  | K     | 1051 | BCR  | C33-C5-C4   | 3.01  | 120.02      | 113.60   |
| 25  | b     | 6045 | BCR  | C38-C26-C27 | 3.01  | 120.02      | 113.60   |
| 25  | B     | 1045 | BCR  | C38-C26-C27 | 3.01  | 120.01      | 113.60   |
| 25  | Z     | 1053 | BCR  | C38-C26-C27 | 3.01  | 120.01      | 113.60   |
| 25  | D     | 1050 | BCR  | C33-C5-C4   | 3.01  | 120.01      | 113.60   |
| 25  | k     | 6052 | BCR  | C33-C5-C4   | 3.01  | 120.01      | 113.60   |
| 25  | C     | 1052 | BCR  | C33-C5-C4   | 3.00  | 119.99      | 113.60   |
| 25  | d     | 6050 | BCR  | C33-C5-C4   | 3.00  | 119.99      | 113.60   |
| 25  | A     | 1044 | BCR  | C28-C27-C26 | -3.00 | 108.71      | 114.06   |
| 25  | H     | 1049 | BCR  | C33-C5-C4   | 3.00  | 119.98      | 113.60   |
| 25  | h     | 6049 | BCR  | C33-C5-C4   | 2.99  | 119.98      | 113.60   |
| 25  | K     | 1051 | BCR  | C38-C26-C27 | 2.99  | 119.97      | 113.60   |
| 25  | a     | 6044 | BCR  | C28-C27-C26 | -2.99 | 108.72      | 114.06   |
| 25  | k     | 6051 | BCR  | C38-C26-C27 | 2.99  | 119.97      | 113.60   |
| 22  | b     | 6023 | CLA  | CAC-C3C-C4C | 2.99  | 128.68      | 124.79   |
| 22  | C     | 1030 | CLA  | CMB-C2B-C1B | 2.98  | 129.96      | 125.42   |
| 22  | c     | 6030 | CLA  | CMB-C2B-C1B | 2.98  | 129.95      | 125.42   |
| 25  | t     | 1046 | BCR  | C30-C25-C26 | -2.98 | 118.57      | 122.64   |
| 22  | B     | 1023 | CLA  | CAC-C3C-C4C | 2.97  | 128.65      | 124.79   |
| 25  | h     | 6049 | BCR  | C38-C26-C27 | 2.97  | 119.92      | 113.60   |
| 25  | H     | 1049 | BCR  | C38-C26-C27 | 2.96  | 119.91      | 113.60   |
| 22  | B     | 1009 | CLA  | CAC-C3C-C4C | 2.96  | 128.64      | 124.79   |
| 22  | B     | 1021 | CLA  | CMB-C2B-C1B | 2.96  | 129.92      | 125.42   |
| 25  | C     | 1054 | BCR  | C38-C26-C27 | 2.95  | 119.89      | 113.60   |
| 22  | b     | 6023 | CLA  | C2D-C1D-ND  | 2.95  | 113.04      | 110.13   |
| 25  | T     | 6046 | BCR  | C30-C25-C26 | -2.95 | 118.61      | 122.64   |
| 25  | c     | 6054 | BCR  | C38-C26-C27 | 2.95  | 119.88      | 113.60   |
| 22  | b     | 6021 | CLA  | CMB-C2B-C1B | 2.94  | 129.90      | 125.42   |
| 22  | b     | 6009 | CLA  | CAC-C3C-C4C | 2.94  | 128.61      | 124.79   |
| 22  | B     | 1023 | CLA  | C2D-C1D-ND  | 2.94  | 113.03      | 110.13   |
| 22  | b     | 6018 | CLA  | C2D-C1D-ND  | 2.94  | 113.03      | 110.13   |
| 22  | a     | 6003 | CLA  | CAC-C3C-C4C | 2.93  | 128.60      | 124.79   |
| 22  | b     | 6015 | CLA  | CAC-C3C-C4C | 2.93  | 128.60      | 124.79   |
| 22  | b     | 6020 | CLA  | C2D-C1D-ND  | 2.93  | 113.03      | 110.13   |
| 25  | a     | 6044 | BCR  | C38-C26-C27 | 2.93  | 119.84      | 113.60   |
| 22  | c     | 6027 | CLA  | C2D-C1D-ND  | 2.92  | 113.02      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1027 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.79   |
| 22  | B     | 1023 | CLA  | CMB-C2B-C1B | 2.92  | 129.87      | 125.42   |
| 22  | A     | 1003 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.79   |
| 22  | c     | 6035 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.79   |
| 22  | b     | 6023 | CLA  | CMB-C2B-C1B | 2.92  | 129.87      | 125.42   |
| 22  | c     | 6026 | CLA  | CMB-C2B-C1B | 2.92  | 129.86      | 125.42   |
| 22  | B     | 1016 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.79   |
| 22  | a     | 6007 | CLA  | CAC-C3C-C4C | 2.92  | 128.58      | 124.79   |
| 22  | H     | 1017 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |
| 22  | B     | 1013 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |
| 22  | K     | 1034 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |
| 22  | B     | 1014 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |
| 22  | a     | 6006 | CLA  | CAC-C3C-C4C | 2.91  | 128.57      | 124.79   |
| 22  | B     | 1018 | CLA  | C2D-C1D-ND  | 2.91  | 113.00      | 110.13   |
| 22  | h     | 6017 | CLA  | CAC-C3C-C4C | 2.91  | 128.57      | 124.79   |
| 22  | b     | 6016 | CLA  | CAC-C3C-C4C | 2.91  | 128.57      | 124.79   |
| 22  | c     | 6029 | CLA  | CMD-C2D-C3D | -2.91 | 121.02      | 127.69   |
| 25  | A     | 1044 | BCR  | C38-C26-C27 | 2.91  | 119.79      | 113.60   |
| 22  | d     | 6008 | CLA  | CMD-C2D-C3D | -2.91 | 121.03      | 127.69   |
| 22  | B     | 1022 | CLA  | CAC-C3C-C4C | 2.90  | 128.57      | 124.79   |
| 22  | C     | 1026 | CLA  | CAC-C3C-C4C | 2.90  | 128.57      | 124.79   |
| 22  | c     | 6026 | CLA  | CAC-C3C-C4C | 2.90  | 128.57      | 124.79   |
| 22  | D     | 1008 | CLA  | CMD-C2D-C3D | -2.90 | 121.03      | 127.69   |
| 22  | k     | 6034 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | C     | 1032 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | C     | 1029 | CLA  | CMD-C2D-C3D | -2.90 | 121.04      | 127.69   |
| 22  | b     | 6014 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | c     | 6027 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | c     | 6028 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | c     | 6032 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | B     | 1020 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | B     | 1024 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | c     | 6025 | CLA  | C2D-C1D-ND  | 2.90  | 112.99      | 110.13   |
| 22  | d     | 6005 | CLA  | CMB-C2B-C1B | 2.90  | 129.83      | 125.42   |
| 22  | C     | 1025 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | D     | 1004 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | b     | 6020 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 22  | C     | 1026 | CLA  | CMB-C2B-C1B | 2.90  | 129.83      | 125.42   |
| 22  | C     | 1035 | CLA  | CAC-C3C-C4C | 2.89  | 128.56      | 124.79   |
| 25  | A     | 1044 | BCR  | C37-C22-C21 | -2.89 | 118.13      | 122.82   |
| 22  | b     | 6022 | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 25  | a     | 6044 | BCR  | C37-C22-C21 | -2.89 | 118.13      | 122.82   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1015 | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 22  | A     | 1006 | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 22  | A     | 1007 | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 22  | c     | 6025 | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 22  | B     | 1020 | CLA  | C2D-C1D-ND  | 2.89  | 112.98      | 110.13   |
| 22  | a     | 6003 | CLA  | C2D-C1D-ND  | 2.89  | 112.98      | 110.13   |
| 22  | B     | 1021 | CLA  | CMD-C2D-C3D | -2.89 | 121.07      | 127.69   |
| 22  | c     | 6027 | CLA  | CMB-C2B-C1B | 2.89  | 129.81      | 125.42   |
| 22  | b     | 6014 | CLA  | CMB-C2B-C1B | 2.88  | 129.81      | 125.42   |
| 22  | C     | 1031 | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.79   |
| 22  | b     | 6013 | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.79   |
| 22  | C     | 1025 | CLA  | C2D-C1D-ND  | 2.88  | 112.98      | 110.13   |
| 22  | C     | 1036 | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.79   |
| 22  | D     | 1005 | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.79   |
| 22  | k     | 6034 | CLA  | CMD-C2D-C3D | -2.88 | 121.08      | 127.69   |
| 22  | B     | 1020 | CLA  | CMB-C2B-C1B | 2.88  | 129.81      | 125.42   |
| 22  | b     | 6021 | CLA  | CMD-C2D-C3D | -2.88 | 121.08      | 127.69   |
| 22  | B     | 1018 | CLA  | CMB-C2B-C1B | 2.88  | 129.80      | 125.42   |
| 22  | b     | 6020 | CLA  | CMB-C2B-C1B | 2.88  | 129.80      | 125.42   |
| 22  | d     | 6005 | CLA  | CAC-C3C-C4C | 2.88  | 128.53      | 124.79   |
| 22  | B     | 1024 | CLA  | CMB-C2B-C1B | 2.88  | 129.80      | 125.42   |
| 22  | c     | 6030 | CLA  | C2D-C1D-ND  | 2.88  | 112.97      | 110.13   |
| 22  | B     | 1012 | CLA  | CAC-C3C-C4C | 2.88  | 128.53      | 124.79   |
| 22  | C     | 1037 | CLA  | CAC-C3C-C4C | 2.88  | 128.53      | 124.79   |
| 22  | c     | 6036 | CLA  | C2D-C1D-ND  | 2.88  | 112.97      | 110.13   |
| 22  | C     | 1029 | CLA  | CMB-C2B-C1B | 2.88  | 129.80      | 125.42   |
| 22  | d     | 6004 | CLA  | CMB-C2B-C1B | 2.87  | 129.80      | 125.42   |
| 22  | h     | 6017 | CLA  | CMB-C2B-C1B | 2.87  | 129.80      | 125.42   |
| 22  | C     | 1028 | CLA  | CAC-C3C-C4C | 2.87  | 128.53      | 124.79   |
| 22  | B     | 1021 | CLA  | C2D-C1D-ND  | 2.87  | 112.97      | 110.13   |
| 22  | b     | 6016 | CLA  | C2D-C1D-ND  | 2.87  | 112.97      | 110.13   |
| 22  | d     | 6004 | CLA  | CAC-C3C-C4C | 2.87  | 128.53      | 124.79   |
| 22  | c     | 6035 | CLA  | CMD-C2D-C3D | -2.87 | 121.10      | 127.69   |
| 22  | B     | 1014 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 22  | C     | 1033 | CLA  | CAC-C3C-C4C | 2.87  | 128.53      | 124.79   |
| 22  | c     | 6026 | CLA  | CMD-C2D-C3D | -2.87 | 121.10      | 127.69   |
| 22  | h     | 6017 | CLA  | C2D-C1D-ND  | 2.87  | 112.97      | 110.13   |
| 22  | B     | 1019 | CLA  | CAC-C3C-C4C | 2.87  | 128.53      | 124.79   |
| 22  | A     | 1003 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 22  | b     | 6015 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 22  | b     | 6018 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 22  | b     | 6024 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | k     | 6034 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 22  | b     | 6019 | CLA  | CAC-C3C-C4C | 2.87  | 128.52      | 124.79   |
| 22  | A     | 1003 | CLA  | C2D-C1D-ND  | 2.87  | 112.97      | 110.13   |
| 22  | C     | 1027 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 22  | b     | 6016 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 22  | B     | 1018 | CLA  | CAC-C3C-C4C | 2.87  | 128.52      | 124.79   |
| 22  | c     | 6036 | CLA  | CAC-C3C-C4C | 2.87  | 128.52      | 124.79   |
| 22  | C     | 1025 | CLA  | CMB-C2B-C1B | 2.87  | 129.78      | 125.42   |
| 22  | A     | 1003 | CLA  | CMD-C2D-C3D | -2.87 | 121.11      | 127.69   |
| 22  | b     | 6012 | CLA  | CAC-C3C-C4C | 2.87  | 128.52      | 124.79   |
| 22  | K     | 1034 | CLA  | CMB-C2B-C1B | 2.87  | 129.78      | 125.42   |
| 22  | c     | 6029 | CLA  | CMB-C2B-C1B | 2.87  | 129.78      | 125.42   |
| 22  | b     | 6011 | CLA  | C4C-C3C-C2C | -2.87 | 102.72      | 106.89   |
| 22  | B     | 1016 | CLA  | CMB-C2B-C1B | 2.86  | 129.78      | 125.42   |
| 22  | D     | 1004 | CLA  | CMB-C2B-C1B | 2.86  | 129.78      | 125.42   |
| 22  | C     | 1036 | CLA  | C2D-C1D-ND  | 2.86  | 112.96      | 110.13   |
| 22  | D     | 1005 | CLA  | CMB-C2B-C1B | 2.86  | 129.78      | 125.42   |
| 22  | c     | 6035 | CLA  | CMB-C2B-C1B | 2.86  | 129.78      | 125.42   |
| 22  | b     | 6023 | CLA  | CMD-C2D-C3D | -2.86 | 121.12      | 127.69   |
| 22  | B     | 1014 | CLA  | C2D-C1D-ND  | 2.86  | 112.96      | 110.13   |
| 22  | B     | 1015 | CLA  | C2D-C1D-ND  | 2.86  | 112.96      | 110.13   |
| 22  | C     | 1030 | CLA  | C2D-C1D-ND  | 2.86  | 112.96      | 110.13   |
| 22  | A     | 1007 | CLA  | CMB-C2B-C1B | 2.86  | 129.78      | 125.42   |
| 22  | c     | 6033 | CLA  | CAC-C3C-C4C | 2.86  | 128.51      | 124.79   |
| 22  | c     | 6028 | CLA  | CMB-C2B-C1B | 2.86  | 129.78      | 125.42   |
| 22  | C     | 1033 | CLA  | CMD-C2D-C3D | -2.86 | 121.12      | 127.69   |
| 22  | a     | 6003 | CLA  | CMD-C2D-C3D | -2.86 | 121.12      | 127.69   |
| 22  | C     | 1027 | CLA  | C2D-C1D-ND  | 2.86  | 112.96      | 110.13   |
| 22  | c     | 6037 | CLA  | CMB-C2B-C1B | 2.86  | 129.77      | 125.42   |
| 22  | K     | 1034 | CLA  | CMD-C2D-C3D | -2.86 | 121.13      | 127.69   |
| 22  | D     | 1008 | CLA  | O1D-CGD-CBD | -2.86 | 118.88      | 124.52   |
| 22  | c     | 6036 | CLA  | CMB-C2B-C1B | 2.86  | 129.77      | 125.42   |
| 22  | b     | 6024 | CLA  | CMD-C2D-C3D | -2.86 | 121.13      | 127.69   |
| 22  | C     | 1036 | CLA  | CMB-C2B-C1B | 2.86  | 129.77      | 125.42   |
| 22  | C     | 1031 | CLA  | C2D-C1D-ND  | 2.86  | 112.95      | 110.13   |
| 22  | K     | 1034 | CLA  | C2D-C1D-ND  | 2.86  | 112.95      | 110.13   |
| 22  | b     | 6012 | CLA  | C2D-C1D-ND  | 2.86  | 112.95      | 110.13   |
| 22  | H     | 1017 | CLA  | CMB-C2B-C1B | 2.86  | 129.77      | 125.42   |
| 22  | B     | 1015 | CLA  | CMD-C2D-C3D | -2.86 | 121.14      | 127.69   |
| 22  | b     | 6018 | CLA  | CMD-C2D-C3D | -2.86 | 121.14      | 127.69   |
| 22  | d     | 6004 | CLA  | C2D-C1D-ND  | 2.86  | 112.95      | 110.13   |
| 22  | c     | 6033 | CLA  | CMD-C2D-C3D | -2.86 | 121.14      | 127.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6013 | CLA  | CMB-C2B-C1B | 2.85  | 129.77      | 125.42   |
| 22  | C     | 1035 | CLA  | CMD-C2D-C3D | -2.85 | 121.14      | 127.69   |
| 22  | B     | 1020 | CLA  | CMD-C2D-C3D | -2.85 | 121.14      | 127.69   |
| 22  | B     | 1015 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | C     | 1026 | CLA  | CMD-C2D-C3D | -2.85 | 121.14      | 127.69   |
| 22  | c     | 6026 | CLA  | C2D-C1D-ND  | 2.85  | 112.95      | 110.13   |
| 22  | c     | 6030 | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 22  | a     | 6003 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | B     | 1024 | CLA  | CMD-C2D-C3D | -2.85 | 121.15      | 127.69   |
| 22  | C     | 1031 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | c     | 6031 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | A     | 1007 | CLA  | C2D-C1D-ND  | 2.85  | 112.95      | 110.13   |
| 22  | a     | 6007 | CLA  | C2D-C1D-ND  | 2.85  | 112.95      | 110.13   |
| 22  | C     | 1032 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | b     | 6015 | CLA  | CMD-C2D-C3D | -2.85 | 121.15      | 127.69   |
| 22  | c     | 6037 | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 22  | d     | 6005 | CLA  | CMD-C2D-C3D | -2.85 | 121.15      | 127.69   |
| 22  | b     | 6019 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | C     | 1033 | CLA  | C2D-C1D-ND  | 2.85  | 112.95      | 110.13   |
| 22  | k     | 6034 | CLA  | C2D-C1D-ND  | 2.85  | 112.95      | 110.13   |
| 22  | B     | 1012 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | C     | 1035 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | C     | 1037 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | c     | 6025 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | B     | 1013 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 22  | B     | 1023 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | B     | 1019 | CLA  | CMB-C2B-C1B | 2.85  | 129.75      | 125.42   |
| 22  | b     | 6012 | CLA  | CMB-C2B-C1B | 2.85  | 129.75      | 125.42   |
| 22  | A     | 1007 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | C     | 1031 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | c     | 6032 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | B     | 1018 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | B     | 1022 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | C     | 1025 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | b     | 6022 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | c     | 6025 | CLA  | CMD-C2D-C3D | -2.85 | 121.16      | 127.69   |
| 22  | c     | 6031 | CLA  | CAC-C3C-C4C | 2.85  | 128.49      | 124.79   |
| 22  | b     | 6018 | CLA  | CAC-C3C-C4C | 2.85  | 128.49      | 124.79   |
| 22  | C     | 1026 | CLA  | C2D-C1D-ND  | 2.85  | 112.94      | 110.13   |
| 22  | c     | 6031 | CLA  | C2D-C1D-ND  | 2.85  | 112.94      | 110.13   |
| 22  | B     | 1013 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | D     | 1005 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6020 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | D     | 1005 | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | D     | 1004 | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | b     | 6015 | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | b     | 6021 | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | c     | 6032 | CLA  | CMB-C2B-C1B | 2.84  | 129.75      | 125.42   |
| 22  | c     | 6031 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | B     | 1014 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | b     | 6012 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | a     | 6006 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | b     | 6019 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | B     | 1012 | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | c     | 6035 | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | b     | 6009 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 22  | c     | 6027 | CLA  | CMD-C2D-C3D | -2.84 | 121.18      | 127.69   |
| 22  | H     | 1017 | CLA  | CMD-C2D-C3D | -2.84 | 121.18      | 127.69   |
| 22  | C     | 1028 | CLA  | CMB-C2B-C1B | 2.84  | 129.74      | 125.42   |
| 22  | b     | 6022 | CLA  | CMB-C2B-C1B | 2.84  | 129.74      | 125.42   |
| 22  | C     | 1032 | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | C     | 1027 | CLA  | CMD-C2D-C3D | -2.84 | 121.18      | 127.69   |
| 22  | a     | 6007 | CLA  | CMB-C2B-C1B | 2.84  | 129.74      | 125.42   |
| 22  | C     | 1029 | CLA  | C4-C3-C5    | 2.84  | 120.15      | 115.23   |
| 22  | B     | 1016 | CLA  | CMD-C2D-C3D | -2.84 | 121.18      | 127.69   |
| 22  | c     | 6028 | CLA  | CMD-C2D-C3D | -2.84 | 121.18      | 127.69   |
| 22  | b     | 6024 | CLA  | CAC-C3C-C4C | 2.84  | 128.48      | 124.79   |
| 22  | C     | 1028 | CLA  | CMD-C2D-C3D | -2.84 | 121.19      | 127.69   |
| 22  | B     | 1009 | CLA  | CMD-C2D-C3D | -2.84 | 121.19      | 127.69   |
| 22  | B     | 1011 | CLA  | C4C-C3C-C2C | -2.83 | 102.77      | 106.89   |
| 22  | C     | 1037 | CLA  | C2D-C1D-ND  | 2.83  | 112.93      | 110.13   |
| 22  | d     | 6008 | CLA  | O1D-CGD-CBD | -2.83 | 118.93      | 124.52   |
| 22  | A     | 1006 | CLA  | CMD-C2D-C3D | -2.83 | 121.19      | 127.69   |
| 22  | B     | 1012 | CLA  | CMD-C2D-C3D | -2.83 | 121.19      | 127.69   |
| 22  | c     | 6033 | CLA  | CMB-C2B-C1B | 2.83  | 129.73      | 125.42   |
| 22  | B     | 1019 | CLA  | CMD-C2D-C3D | -2.83 | 121.19      | 127.69   |
| 22  | b     | 6014 | CLA  | CMD-C2D-C3D | -2.83 | 121.19      | 127.69   |
| 22  | B     | 1022 | CLA  | CMB-C2B-C1B | 2.83  | 129.73      | 125.42   |
| 22  | a     | 6006 | CLA  | CMB-C2B-C1B | 2.83  | 129.73      | 125.42   |
| 22  | C     | 1032 | CLA  | CMD-C2D-C3D | -2.83 | 121.20      | 127.69   |
| 22  | b     | 6011 | CLA  | C2D-C1D-ND  | 2.83  | 112.93      | 110.13   |
| 22  | a     | 6007 | CLA  | CMD-C2D-C3D | -2.83 | 121.20      | 127.69   |
| 22  | C     | 1036 | CLA  | CMD-C2D-C3D | -2.83 | 121.20      | 127.69   |
| 22  | b     | 6016 | CLA  | CMD-C2D-C3D | -2.83 | 121.20      | 127.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | c     | 6037 | CLA  | CMD-C2D-C3D | -2.83 | 121.20      | 127.69   |
| 22  | B     | 1010 | CLA  | C2D-C1D-ND  | 2.83  | 112.92      | 110.13   |
| 22  | b     | 6022 | CLA  | C2D-C1D-ND  | 2.83  | 112.92      | 110.13   |
| 22  | A     | 1006 | CLA  | CMB-C2B-C1B | 2.83  | 129.72      | 125.42   |
| 22  | c     | 6029 | CLA  | C4-C3-C5    | 2.83  | 120.14      | 115.23   |
| 22  | b     | 6021 | CLA  | CAC-C3C-C4C | 2.83  | 128.47      | 124.79   |
| 22  | C     | 1037 | CLA  | CMD-C2D-C3D | -2.83 | 121.21      | 127.69   |
| 25  | C     | 1052 | BCR  | C38-C26-C25 | -2.83 | 121.40      | 124.48   |
| 22  | h     | 6017 | CLA  | CMD-C2D-C3D | -2.83 | 121.21      | 127.69   |
| 22  | C     | 1030 | CLA  | O2D-CGD-O1D | -2.83 | 118.35      | 123.85   |
| 22  | B     | 1024 | CLA  | C2D-C1D-ND  | 2.83  | 112.92      | 110.13   |
| 22  | C     | 1033 | CLA  | CMB-C2B-C1B | 2.82  | 129.72      | 125.42   |
| 22  | b     | 6013 | CLA  | CMD-C2D-C3D | -2.82 | 121.21      | 127.69   |
| 22  | B     | 1022 | CLA  | C2D-C1D-ND  | 2.82  | 112.92      | 110.13   |
| 22  | D     | 1004 | CLA  | CMD-C2D-C3D | -2.82 | 121.22      | 127.69   |
| 22  | B     | 1016 | CLA  | C2D-C1D-ND  | 2.82  | 112.92      | 110.13   |
| 25  | B     | 1048 | BCR  | C28-C27-C26 | -2.82 | 109.03      | 114.06   |
| 22  | C     | 1035 | CLA  | C2D-C1D-ND  | 2.82  | 112.92      | 110.13   |
| 22  | B     | 1011 | CLA  | C2D-C1D-ND  | 2.82  | 112.92      | 110.13   |
| 25  | A     | 1044 | BCR  | C23-C24-C25 | 2.82  | 134.53      | 127.00   |
| 25  | k     | 6052 | BCR  | C38-C26-C25 | -2.82 | 121.41      | 124.48   |
| 22  | C     | 1029 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 22  | H     | 1017 | CLA  | C2D-C1D-ND  | 2.82  | 112.91      | 110.13   |
| 25  | a     | 6044 | BCR  | C23-C24-C25 | 2.82  | 134.52      | 127.00   |
| 22  | C     | 1030 | CLA  | CMD-C2D-C3D | -2.82 | 121.23      | 127.69   |
| 22  | B     | 1019 | CLA  | C2D-C1D-ND  | 2.81  | 112.91      | 110.13   |
| 22  | d     | 6005 | CLA  | C2D-C1D-ND  | 2.81  | 112.91      | 110.13   |
| 22  | d     | 6004 | CLA  | CMD-C2D-C3D | -2.81 | 121.24      | 127.69   |
| 25  | T     | 6048 | BCR  | C28-C27-C26 | -2.81 | 109.04      | 114.06   |
| 22  | b     | 6019 | CLA  | C2D-C1D-ND  | 2.81  | 112.91      | 110.13   |
| 22  | c     | 6036 | CLA  | CMD-C2D-C3D | -2.81 | 121.24      | 127.69   |
| 22  | b     | 6010 | CLA  | CMD-C2D-C3D | -2.81 | 121.24      | 127.69   |
| 22  | B     | 1021 | CLA  | CAC-C3C-C4C | 2.81  | 128.45      | 124.79   |
| 22  | c     | 6028 | CLA  | C2D-C1D-ND  | 2.81  | 112.91      | 110.13   |
| 22  | c     | 6037 | CLA  | C2D-C1D-ND  | 2.81  | 112.91      | 110.13   |
| 22  | A     | 1006 | CLA  | C2D-C1D-ND  | 2.81  | 112.91      | 110.13   |
| 22  | b     | 6014 | CLA  | C2D-C1D-ND  | 2.81  | 112.91      | 110.13   |
| 22  | b     | 6010 | CLA  | C2D-C1D-ND  | 2.80  | 112.90      | 110.13   |
| 22  | c     | 6030 | CLA  | CMD-C2D-C3D | -2.80 | 121.26      | 127.69   |
| 25  | a     | 6044 | BCR  | C3-C4-C5    | -2.80 | 109.06      | 114.06   |
| 22  | c     | 6029 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 22  | a     | 6006 | CLA  | C2D-C1D-ND  | 2.80  | 112.90      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1028 | CLA  | C2D-C1D-ND  | 2.80  | 112.90      | 110.13   |
| 22  | d     | 6008 | CLA  | C2D-C1D-ND  | 2.80  | 112.90      | 110.13   |
| 22  | c     | 6032 | CLA  | C2D-C1D-ND  | 2.80  | 112.90      | 110.13   |
| 22  | B     | 1010 | CLA  | CMD-C2D-C3D | -2.80 | 121.27      | 127.69   |
| 22  | b     | 6009 | CLA  | CMB-C2B-C1B | 2.80  | 129.68      | 125.42   |
| 22  | b     | 6024 | CLA  | C2D-C1D-ND  | 2.79  | 112.89      | 110.13   |
| 22  | B     | 1010 | CLA  | C4-C3-C5    | 2.79  | 120.08      | 115.23   |
| 22  | c     | 6033 | CLA  | C2D-C1D-ND  | 2.79  | 112.89      | 110.13   |
| 25  | B     | 1047 | BCR  | C28-C27-C26 | -2.79 | 109.08      | 114.06   |
| 22  | a     | 6003 | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 25  | A     | 1044 | BCR  | C3-C4-C5    | -2.79 | 109.08      | 114.06   |
| 22  | b     | 6013 | CLA  | C4-C3-C5    | 2.79  | 120.07      | 115.23   |
| 23  | d     | 6039 | PHO  | C4-C3-C5    | 2.79  | 120.06      | 115.23   |
| 22  | b     | 6013 | CLA  | C2D-C1D-ND  | 2.79  | 112.88      | 110.13   |
| 22  | B     | 1009 | CLA  | CMB-C2B-C1B | 2.78  | 129.65      | 125.42   |
| 22  | c     | 6032 | CLA  | C4C-C3C-C2C | -2.78 | 102.84      | 106.89   |
| 22  | a     | 6007 | CLA  | C4-C3-C5    | 2.78  | 120.06      | 115.23   |
| 22  | A     | 1007 | CLA  | C4-C3-C5    | 2.78  | 120.05      | 115.23   |
| 22  | b     | 6010 | CLA  | C4-C3-C5    | 2.78  | 120.05      | 115.23   |
| 22  | B     | 1009 | CLA  | C2D-C1D-ND  | 2.78  | 112.88      | 110.13   |
| 22  | C     | 1029 | CLA  | C4C-C3C-C2C | -2.78 | 102.85      | 106.89   |
| 25  | b     | 6047 | BCR  | C28-C27-C26 | -2.78 | 109.10      | 114.06   |
| 22  | B     | 1011 | CLA  | CHB-C4A-NA  | 2.78  | 128.41      | 124.40   |
| 22  | b     | 6021 | CLA  | C4-C3-C5    | 2.78  | 120.05      | 115.23   |
| 22  | B     | 1013 | CLA  | C2D-C1D-ND  | 2.77  | 112.87      | 110.13   |
| 22  | D     | 1008 | CLA  | C4-C3-C5    | 2.77  | 120.04      | 115.23   |
| 22  | A     | 1003 | CLA  | C4C-C3C-C2C | -2.77 | 102.85      | 106.89   |
| 22  | b     | 6009 | CLA  | C4C-C3C-C2C | -2.77 | 102.85      | 106.89   |
| 22  | b     | 6014 | CLA  | C4-C3-C5    | 2.77  | 120.04      | 115.23   |
| 22  | B     | 1021 | CLA  | C4-C3-C5    | 2.77  | 120.04      | 115.23   |
| 22  | B     | 1015 | CLA  | C4-C3-C5    | 2.77  | 120.04      | 115.23   |
| 24  | d     | 6042 | PQ9  | C29-C28-C30 | 2.77  | 120.04      | 115.23   |
| 22  | d     | 6004 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 22  | C     | 1029 | CLA  | C2D-C1D-ND  | 2.77  | 112.87      | 110.13   |
| 22  | c     | 6035 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 24  | D     | 1042 | PQ9  | C19-C18-C20 | 2.77  | 120.04      | 115.23   |
| 22  | B     | 1021 | CLA  | CHB-C4A-NA  | 2.77  | 128.40      | 124.40   |
| 22  | B     | 1013 | CLA  | C4-C3-C5    | 2.77  | 120.04      | 115.23   |
| 22  | d     | 6008 | CLA  | C4-C3-C5    | 2.77  | 120.04      | 115.23   |
| 22  | B     | 1009 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 22  | c     | 6028 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 22  | c     | 6029 | CLA  | C2D-C1D-ND  | 2.77  | 112.87      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | H     | 1017 | CLA  | C4-C3-C5    | 2.77  | 120.03      | 115.23   |
| 23  | D     | 1039 | PHO  | C4-C3-C5    | 2.77  | 120.03      | 115.23   |
| 22  | b     | 6015 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 24  | d     | 6042 | PQ9  | C19-C18-C20 | 2.77  | 120.03      | 115.23   |
| 22  | C     | 1035 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 22  | B     | 1010 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 22  | C     | 1032 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 22  | B     | 1013 | CLA  | C4C-C3C-C2C | -2.77 | 102.87      | 106.89   |
| 22  | C     | 1036 | CLA  | C4-C3-C5    | 2.77  | 120.03      | 115.23   |
| 25  | T     | 6046 | BCR  | C38-C26-C27 | 2.77  | 119.49      | 113.60   |
| 22  | b     | 6009 | CLA  | C2D-C1D-ND  | 2.76  | 112.86      | 110.13   |
| 24  | d     | 6042 | PQ9  | C39-C38-C40 | 2.76  | 120.03      | 115.23   |
| 24  | a     | 6043 | PQ9  | C39-C38-C40 | 2.76  | 120.02      | 115.23   |
| 22  | B     | 1011 | CLA  | CMD-C2D-C3D | -2.76 | 121.35      | 127.69   |
| 22  | b     | 6010 | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.89   |
| 22  | D     | 1004 | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.89   |
| 22  | b     | 6015 | CLA  | C4-C3-C5    | 2.76  | 120.02      | 115.23   |
| 24  | D     | 1042 | PQ9  | C39-C38-C40 | 2.76  | 120.02      | 115.23   |
| 24  | D     | 1042 | PQ9  | C29-C28-C30 | 2.76  | 120.02      | 115.23   |
| 22  | B     | 1024 | CLA  | C4-C3-C5    | 2.76  | 120.02      | 115.23   |
| 22  | b     | 6022 | CLA  | C4-C3-C5    | 2.76  | 120.02      | 115.23   |
| 24  | d     | 6042 | PQ9  | C34-C33-C35 | 2.76  | 120.02      | 115.23   |
| 22  | C     | 1026 | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.89   |
| 22  | b     | 6021 | CLA  | CHB-C4A-NA  | 2.76  | 128.38      | 124.40   |
| 25  | t     | 1046 | BCR  | C38-C26-C27 | 2.76  | 119.48      | 113.60   |
| 22  | D     | 1004 | CLA  | C4-C3-C5    | 2.76  | 120.02      | 115.23   |
| 22  | c     | 6032 | CLA  | C4-C3-C5    | 2.76  | 120.02      | 115.23   |
| 24  | D     | 1042 | PQ9  | C24-C23-C25 | 2.76  | 120.02      | 115.23   |
| 24  | d     | 6042 | PQ9  | C24-C23-C25 | 2.76  | 120.02      | 115.23   |
| 22  | C     | 1028 | CLA  | C4C-C3C-C2C | -2.76 | 102.88      | 106.89   |
| 22  | c     | 6037 | CLA  | C4C-C3C-C2C | -2.76 | 102.88      | 106.89   |
| 22  | c     | 6026 | CLA  | C4-C3-C5    | 2.76  | 120.02      | 115.23   |
| 22  | C     | 1031 | CLA  | C4C-C3C-C2C | -2.76 | 102.88      | 106.89   |
| 22  | d     | 6005 | CLA  | CHB-C4A-NA  | 2.76  | 128.38      | 124.40   |
| 22  | k     | 6034 | CLA  | C4-C3-C5    | 2.76  | 120.01      | 115.23   |
| 24  | A     | 1043 | PQ9  | C14-C13-C15 | 2.76  | 120.01      | 115.23   |
| 22  | C     | 1027 | CLA  | C4C-C3C-C2C | -2.76 | 102.88      | 106.89   |
| 23  | A     | 1038 | PHO  | C4-C3-C5    | 2.76  | 120.01      | 115.23   |
| 22  | B     | 1023 | CLA  | C4-C3-C5    | 2.75  | 120.01      | 115.23   |
| 24  | a     | 6043 | PQ9  | C14-C13-C15 | 2.75  | 120.01      | 115.23   |
| 22  | b     | 6016 | CLA  | C4C-C3C-C2C | -2.75 | 102.88      | 106.89   |
| 22  | c     | 6025 | CLA  | C4C-C3C-C2C | -2.75 | 102.88      | 106.89   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | D     | 1042 | PQ9  | C14-C13-C15 | 2.75  | 120.01      | 115.23   |
| 22  | B     | 1022 | CLA  | C4C-C3C-C2C | -2.75 | 102.88      | 106.89   |
| 22  | C     | 1037 | CLA  | C4C-C3C-C2C | -2.75 | 102.88      | 106.89   |
| 22  | h     | 6017 | CLA  | C4-C3-C5    | 2.75  | 120.01      | 115.23   |
| 22  | a     | 6006 | CLA  | C4-C3-C5    | 2.75  | 120.01      | 115.23   |
| 22  | d     | 6004 | CLA  | C4-C3-C5    | 2.75  | 120.01      | 115.23   |
| 22  | A     | 1006 | CLA  | C4-C3-C5    | 2.75  | 120.01      | 115.23   |
| 22  | A     | 1003 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 24  | A     | 1043 | PQ9  | C39-C38-C40 | 2.75  | 120.00      | 115.23   |
| 22  | b     | 6020 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | c     | 6033 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | b     | 6011 | CLA  | CMD-C2D-C3D | -2.75 | 121.38      | 127.69   |
| 22  | c     | 6031 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 24  | a     | 6043 | PQ9  | C24-C23-C25 | 2.75  | 120.00      | 115.23   |
| 22  | B     | 1016 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | B     | 1024 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | a     | 6003 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 22  | B     | 1014 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 22  | C     | 1032 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 22  | B     | 1014 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | K     | 1034 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | C     | 1026 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 22  | c     | 6037 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 22  | B     | 1010 | CLA  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 22  | C     | 1025 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | h     | 6017 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | a     | 6006 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | B     | 1018 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 22  | c     | 6027 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 23  | D     | 1039 | PHO  | O2A-CGA-CBA | 2.75  | 120.21      | 111.83   |
| 22  | C     | 1033 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | b     | 6022 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | C     | 1031 | CLA  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 23  | d     | 6039 | PHO  | O2A-CGA-CBA | 2.75  | 120.21      | 111.83   |
| 22  | c     | 6031 | CLA  | CHB-C4A-NA  | 2.75  | 128.36      | 124.40   |
| 22  | c     | 6029 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | C     | 1033 | CLA  | C4-C3-C5    | 2.75  | 119.99      | 115.23   |
| 22  | b     | 6011 | CLA  | C4-C3-C5    | 2.75  | 119.99      | 115.23   |
| 22  | b     | 6018 | CLA  | C4-C3-C5    | 2.75  | 119.99      | 115.23   |
| 22  | b     | 6014 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 22  | b     | 6010 | CLA  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 22  | B     | 1011 | CLA  | C4-C3-C5    | 2.75  | 119.99      | 115.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1027 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 28  | B     | 1060 | MGE  | O1G-C1A-C2A | 2.74  | 120.20      | 111.83   |
| 28  | D     | 1062 | MGE  | O1G-C1A-C2A | 2.74  | 120.20      | 111.83   |
| 22  | b     | 6013 | CLA  | C4C-C3C-C2C | -2.74 | 102.90      | 106.89   |
| 26  | A     | 1063 | LHG  | O8-C23-C24  | 2.74  | 120.20      | 111.83   |
| 29  | c     | 6055 | DGD  | O1G-C1A-C2A | 2.74  | 120.20      | 111.83   |
| 29  | C     | 1055 | DGD  | O1G-C1A-C2A | 2.74  | 120.20      | 111.83   |
| 22  | C     | 1035 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 22  | B     | 1015 | CLA  | C4C-C3C-C2C | -2.74 | 102.90      | 106.89   |
| 22  | b     | 6011 | CLA  | CHB-C4A-NA  | 2.74  | 128.36      | 124.40   |
| 22  | K     | 1034 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 24  | a     | 6043 | PQ9  | C19-C18-C20 | 2.74  | 119.99      | 115.23   |
| 22  | B     | 1012 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 22  | B     | 1020 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 22  | B     | 1022 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 22  | b     | 6024 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 22  | c     | 6036 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 22  | B     | 1018 | CLA  | C4C-C3C-C2C | -2.74 | 102.90      | 106.89   |
| 22  | b     | 6019 | CLA  | CHB-C4A-NA  | 2.74  | 128.36      | 124.40   |
| 22  | c     | 6035 | CLA  | C4-C3-C5    | 2.74  | 119.99      | 115.23   |
| 24  | A     | 1043 | PQ9  | C19-C18-C20 | 2.74  | 119.99      | 115.23   |
| 22  | b     | 6023 | CLA  | C4-C3-C5    | 2.74  | 119.98      | 115.23   |
| 24  | A     | 1043 | PQ9  | C24-C23-C25 | 2.74  | 119.98      | 115.23   |
| 22  | D     | 1008 | CLA  | C2D-C1D-ND  | 2.74  | 112.84      | 110.13   |
| 28  | b     | 6060 | MGE  | O1G-C1A-C2A | 2.74  | 120.19      | 111.83   |
| 22  | B     | 1019 | CLA  | CHB-C4A-NA  | 2.74  | 128.35      | 124.40   |
| 22  | C     | 1036 | CLA  | C4C-C3C-C2C | -2.74 | 102.90      | 106.89   |
| 22  | c     | 6033 | CLA  | C4-C3-C5    | 2.74  | 119.98      | 115.23   |
| 22  | C     | 1030 | CLA  | CHB-C4A-NA  | 2.74  | 128.35      | 124.40   |
| 22  | B     | 1019 | CLA  | C4-C3-C5    | 2.74  | 119.98      | 115.23   |
| 29  | b     | 6058 | DGD  | O1G-C1A-C2A | 2.74  | 120.19      | 111.83   |
| 22  | H     | 1017 | CLA  | C4C-C3C-C2C | -2.74 | 102.91      | 106.89   |
| 29  | C     | 1056 | DGD  | O1G-C1A-C2A | 2.74  | 120.18      | 111.83   |
| 22  | b     | 6020 | CLA  | C4-C3-C5    | 2.74  | 119.98      | 115.23   |
| 24  | D     | 1042 | PQ9  | C34-C33-C35 | 2.74  | 119.98      | 115.23   |
| 22  | c     | 6030 | CLA  | C4C-C3C-C2C | -2.74 | 102.91      | 106.89   |
| 23  | A     | 1038 | PHO  | O2A-CGA-CBA | 2.74  | 120.17      | 111.83   |
| 28  | D     | 1059 | MGE  | O1G-C1A-C2A | 2.74  | 120.17      | 111.83   |
| 22  | D     | 1005 | CLA  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 22  | C     | 1029 | CLA  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 23  | a     | 6038 | PHO  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 29  | B     | 1058 | DGD  | O1G-C1A-C2A | 2.73  | 120.17      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6014 | CLA  | CHB-C4A-NA  | 2.73  | 128.35      | 124.40   |
| 23  | a     | 6038 | PHO  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 22  | B     | 1020 | CLA  | C4C-C3C-C2C | -2.73 | 102.91      | 106.89   |
| 28  | l     | 6061 | MGE  | O1G-C1A-C2A | 2.73  | 120.17      | 111.83   |
| 22  | d     | 6005 | CLA  | C4C-C3C-C2C | -2.73 | 102.91      | 106.89   |
| 26  | a     | 6063 | LHG  | O8-C23-C24  | 2.73  | 120.17      | 111.83   |
| 22  | C     | 1037 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 22  | c     | 6029 | CLA  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 28  | L     | 1061 | MGE  | O1G-C1A-C2A | 2.73  | 120.17      | 111.83   |
| 28  | d     | 6062 | MGE  | O1G-C1A-C2A | 2.73  | 120.17      | 111.83   |
| 22  | c     | 6027 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 24  | A     | 1043 | PQ9  | C29-C28-C30 | 2.73  | 119.97      | 115.23   |
| 24  | A     | 1043 | PQ9  | C34-C33-C35 | 2.73  | 119.97      | 115.23   |
| 22  | C     | 1030 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 22  | c     | 6027 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 22  | c     | 6031 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 22  | c     | 6036 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 22  | c     | 6033 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 22  | b     | 6012 | CLA  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 22  | D     | 1005 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 22  | B     | 1012 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 29  | c     | 6056 | DGD  | O1G-C1A-C2A | 2.73  | 120.16      | 111.83   |
| 22  | C     | 1037 | CLA  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 22  | B     | 1014 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 22  | C     | 1025 | CLA  | C4-C3-C5    | 2.73  | 119.96      | 115.23   |
| 22  | b     | 6015 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 24  | a     | 6043 | PQ9  | C29-C28-C30 | 2.73  | 119.96      | 115.23   |
| 22  | b     | 6009 | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 22  | b     | 6012 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 22  | c     | 6037 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 22  | d     | 6005 | CLA  | C4-C3-C5    | 2.73  | 119.96      | 115.23   |
| 22  | C     | 1028 | CLA  | C4-C3-C5    | 2.73  | 119.96      | 115.23   |
| 22  | b     | 6024 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 24  | d     | 6042 | PQ9  | C14-C13-C15 | 2.73  | 119.96      | 115.23   |
| 22  | c     | 6026 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 22  | k     | 6034 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 22  | B     | 1016 | CLA  | C4-C3-C5    | 2.72  | 119.96      | 115.23   |
| 22  | B     | 1011 | CLA  | CAC-C3C-C4C | 2.72  | 128.34      | 124.79   |
| 22  | A     | 1007 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 22  | b     | 6022 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 22  | c     | 6028 | CLA  | C4-C3-C5    | 2.72  | 119.96      | 115.23   |
| 22  | a     | 6006 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1036 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 22  | b     | 6011 | CLA  | CAC-C3C-C4C | 2.72  | 128.33      | 124.79   |
| 22  | D     | 1005 | CLA  | C4C-C3C-C2C | -2.72 | 102.93      | 106.89   |
| 22  | B     | 1016 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 22  | c     | 6030 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 22  | A     | 1006 | CLA  | C4C-C3C-C2C | -2.72 | 102.93      | 106.89   |
| 22  | b     | 6018 | CLA  | C4C-C3C-C2C | -2.72 | 102.93      | 106.89   |
| 22  | b     | 6016 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 22  | c     | 6035 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 22  | A     | 1007 | CLA  | C4C-C3C-C2C | -2.72 | 102.93      | 106.89   |
| 22  | B     | 1019 | CLA  | C4C-C3C-C2C | -2.72 | 102.93      | 106.89   |
| 22  | c     | 6025 | CLA  | C4-C3-C5    | 2.72  | 119.95      | 115.23   |
| 24  | a     | 6043 | PQ9  | C34-C33-C35 | 2.72  | 119.95      | 115.23   |
| 22  | b     | 6012 | CLA  | C4C-C3C-C2C | -2.72 | 102.93      | 106.89   |
| 29  | C     | 1057 | DGD  | O1G-C1A-C2A | 2.72  | 120.13      | 111.83   |
| 22  | B     | 1012 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 25  | k     | 6052 | BCR  | C37-C22-C21 | -2.72 | 118.41      | 122.82   |
| 28  | d     | 6059 | MGE  | O1G-C1A-C2A | 2.72  | 120.12      | 111.83   |
| 22  | a     | 6003 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 22  | c     | 6036 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 22  | k     | 6034 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 22  | B     | 1023 | CLA  | C4C-C3C-C2C | -2.72 | 102.94      | 106.89   |
| 22  | B     | 1024 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 22  | b     | 6016 | CLA  | C4-C3-C5    | 2.72  | 119.94      | 115.23   |
| 22  | C     | 1031 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 22  | B     | 1009 | CLA  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |
| 22  | B     | 1022 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 22  | b     | 6023 | CLA  | C4C-C3C-C2C | -2.71 | 102.94      | 106.89   |
| 22  | B     | 1020 | CLA  | CHB-C4A-NA  | 2.71  | 128.32      | 124.40   |
| 22  | b     | 6020 | CLA  | CHB-C4A-NA  | 2.71  | 128.32      | 124.40   |
| 22  | c     | 6032 | CLA  | CHB-C4A-NA  | 2.71  | 128.32      | 124.40   |
| 22  | b     | 6019 | CLA  | C4-C3-C5    | 2.71  | 119.94      | 115.23   |
| 22  | b     | 6019 | CLA  | C4C-C3C-C2C | -2.71 | 102.94      | 106.89   |
| 22  | C     | 1035 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | d     | 6008 | CLA  | C4C-C3C-C2C | -2.71 | 102.94      | 106.89   |
| 22  | a     | 6007 | CLA  | C4C-C3C-C2C | -2.71 | 102.94      | 106.89   |
| 22  | B     | 1013 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | A     | 1003 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | b     | 6009 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | h     | 6017 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | A     | 1006 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | C     | 1026 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29  | c     | 6057 | DGD  | O1G-C1A-C2A | 2.71  | 120.09      | 111.83   |
| 22  | B     | 1009 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | B     | 1015 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | C     | 1027 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 22  | b     | 6020 | CLA  | O2A-CGA-CBA | 2.71  | 120.08      | 111.83   |
| 22  | B     | 1021 | CLA  | C4C-C3C-C2C | -2.70 | 102.96      | 106.89   |
| 25  | C     | 1052 | BCR  | C37-C22-C21 | -2.70 | 118.44      | 122.82   |
| 22  | K     | 1034 | CLA  | CHB-C4A-NA  | 2.70  | 128.30      | 124.40   |
| 22  | b     | 6021 | CLA  | C4C-C3C-C2C | -2.70 | 102.96      | 106.89   |
| 22  | c     | 6025 | CLA  | CHB-C4A-NA  | 2.70  | 128.30      | 124.40   |
| 22  | C     | 1033 | CLA  | CHB-C4A-NA  | 2.70  | 128.30      | 124.40   |
| 22  | C     | 1032 | CLA  | CHB-C4A-NA  | 2.70  | 128.30      | 124.40   |
| 22  | D     | 1008 | CLA  | C4C-C3C-C2C | -2.70 | 102.96      | 106.89   |
| 22  | a     | 6007 | CLA  | CHB-C4A-NA  | 2.70  | 128.30      | 124.40   |
| 22  | B     | 1014 | CLA  | O2A-CGA-CBA | 2.70  | 120.06      | 111.83   |
| 22  | c     | 6025 | CLA  | O2A-CGA-CBA | 2.70  | 120.06      | 111.83   |
| 22  | B     | 1020 | CLA  | O2A-CGA-CBA | 2.70  | 120.06      | 111.83   |
| 22  | b     | 6014 | CLA  | O2A-CGA-CBA | 2.70  | 120.06      | 111.83   |
| 22  | A     | 1007 | CLA  | O2A-CGA-CBA | 2.70  | 120.06      | 111.83   |
| 22  | C     | 1025 | CLA  | CHB-C4A-NA  | 2.70  | 128.29      | 124.40   |
| 22  | C     | 1029 | CLA  | O1D-CGD-CBD | -2.70 | 119.20      | 124.52   |
| 22  | h     | 6017 | CLA  | O2A-CGA-CBA | 2.69  | 120.05      | 111.83   |
| 23  | a     | 6038 | PHO  | O1D-CGD-CBD | -2.69 | 120.64      | 124.72   |
| 22  | b     | 6024 | CLA  | CHB-C4A-NA  | 2.69  | 128.29      | 124.40   |
| 22  | C     | 1025 | CLA  | O2A-CGA-CBA | 2.69  | 120.05      | 111.83   |
| 22  | C     | 1033 | CLA  | O2A-CGA-CBA | 2.69  | 120.04      | 111.83   |
| 22  | b     | 6022 | CLA  | O2A-CGA-CBA | 2.69  | 120.04      | 111.83   |
| 22  | D     | 1008 | CLA  | CHB-C4A-NA  | 2.69  | 128.28      | 124.40   |
| 22  | c     | 6029 | CLA  | O1D-CGD-CBD | -2.69 | 119.21      | 124.52   |
| 22  | H     | 1017 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | c     | 6033 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | c     | 6027 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | C     | 1029 | CLA  | CHB-C4A-NA  | 2.69  | 128.28      | 124.40   |
| 22  | H     | 1017 | CLA  | CHB-C4A-NA  | 2.69  | 128.28      | 124.40   |
| 22  | C     | 1027 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | B     | 1016 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | a     | 6007 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | k     | 6034 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | d     | 6008 | CLA  | CHB-C4A-NA  | 2.69  | 128.28      | 124.40   |
| 22  | a     | 6003 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | B     | 1019 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | C     | 1035 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1028 | CLA  | O2A-CGA-CBA | 2.69  | 120.02      | 111.83   |
| 22  | b     | 6010 | CLA  | O2A-CGA-CBA | 2.69  | 120.02      | 111.83   |
| 22  | c     | 6028 | CLA  | O2A-CGA-CBA | 2.69  | 120.02      | 111.83   |
| 22  | B     | 1018 | CLA  | O2A-CGA-CBA | 2.68  | 120.02      | 111.83   |
| 22  | b     | 6016 | CLA  | O2A-CGA-CBA | 2.68  | 120.02      | 111.83   |
| 22  | b     | 6015 | CLA  | O2A-CGA-CBA | 2.68  | 120.02      | 111.83   |
| 22  | B     | 1018 | CLA  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 22  | C     | 1028 | CLA  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 22  | c     | 6035 | CLA  | O2A-CGA-CBA | 2.68  | 120.02      | 111.83   |
| 22  | b     | 6019 | CLA  | O2A-CGA-CBA | 2.68  | 120.02      | 111.83   |
| 22  | c     | 6029 | CLA  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 22  | C     | 1030 | CLA  | C4-C3-C5    | 2.68  | 119.88      | 115.23   |
| 22  | c     | 6026 | CLA  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 22  | d     | 6008 | CLA  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 22  | D     | 1008 | CLA  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 22  | C     | 1032 | CLA  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 22  | c     | 6032 | CLA  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 22  | b     | 6013 | CLA  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 22  | A     | 1003 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 22  | B     | 1012 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 22  | b     | 6013 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 22  | D     | 1004 | CLA  | CHB-C4A-NA  | 2.68  | 128.26      | 124.40   |
| 22  | C     | 1031 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 22  | c     | 6031 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 22  | B     | 1009 | CLA  | C4-C3-C5    | 2.68  | 119.88      | 115.23   |
| 22  | b     | 6009 | CLA  | C4-C3-C5    | 2.68  | 119.87      | 115.23   |
| 22  | B     | 1015 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 22  | B     | 1022 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 22  | B     | 1013 | CLA  | O2A-CGA-CBA | 2.68  | 119.99      | 111.83   |
| 22  | b     | 6010 | CLA  | CHB-C4A-NA  | 2.68  | 128.26      | 124.40   |
| 22  | B     | 1010 | CLA  | O2A-CGA-CBA | 2.68  | 119.99      | 111.83   |
| 22  | K     | 1034 | CLA  | O2A-CGA-CBA | 2.68  | 119.99      | 111.83   |
| 22  | b     | 6012 | CLA  | O2A-CGA-CBA | 2.67  | 119.99      | 111.83   |
| 22  | D     | 1005 | CLA  | O2A-CGA-CBA | 2.67  | 119.99      | 111.83   |
| 22  | c     | 6026 | CLA  | O2A-CGA-CBA | 2.67  | 119.99      | 111.83   |
| 23  | A     | 1038 | PHO  | O1D-CGD-CBD | -2.67 | 120.67      | 124.72   |
| 22  | c     | 6028 | CLA  | CHB-C4A-NA  | 2.67  | 128.26      | 124.40   |
| 22  | B     | 1024 | CLA  | O2A-CGA-CBA | 2.67  | 119.98      | 111.83   |
| 22  | C     | 1026 | CLA  | O2A-CGA-CBA | 2.67  | 119.98      | 111.83   |
| 22  | B     | 1010 | CLA  | CHB-C4A-NA  | 2.67  | 128.25      | 124.40   |
| 22  | C     | 1036 | CLA  | O2A-CGA-CBA | 2.67  | 119.97      | 111.83   |
| 22  | c     | 6030 | CLA  | C4-C3-C5    | 2.67  | 119.86      | 115.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1006 | CLA  | O2A-CGA-CBA | 2.67  | 119.97      | 111.83   |
| 22  | d     | 6005 | CLA  | O2A-CGA-CBA | 2.67  | 119.96      | 111.83   |
| 22  | b     | 6024 | CLA  | O2A-CGA-CBA | 2.67  | 119.96      | 111.83   |
| 22  | d     | 6004 | CLA  | O2A-CGA-CBA | 2.67  | 119.96      | 111.83   |
| 22  | b     | 6018 | CLA  | O2A-CGA-CBA | 2.67  | 119.96      | 111.83   |
| 22  | b     | 6018 | CLA  | CHB-C4A-NA  | 2.66  | 128.25      | 124.40   |
| 22  | d     | 6004 | CLA  | CHB-C4A-NA  | 2.66  | 128.25      | 124.40   |
| 22  | D     | 1004 | CLA  | O2A-CGA-CBA | 2.66  | 119.95      | 111.83   |
| 22  | c     | 6036 | CLA  | O2A-CGA-CBA | 2.66  | 119.95      | 111.83   |
| 22  | b     | 6023 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 22  | b     | 6023 | CLA  | O2D-CGD-O1D | -2.65 | 118.68      | 123.85   |
| 22  | a     | 6006 | CLA  | O2A-CGA-CBA | 2.65  | 119.91      | 111.83   |
| 25  | H     | 1049 | BCR  | C28-C27-C26 | -2.65 | 109.33      | 114.06   |
| 22  | B     | 1023 | CLA  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 22  | C     | 1037 | CLA  | O2A-CGA-CBA | 2.65  | 119.91      | 111.83   |
| 22  | c     | 6037 | CLA  | O2A-CGA-CBA | 2.65  | 119.90      | 111.83   |
| 23  | D     | 1039 | PHO  | O1D-CGD-CBD | -2.64 | 120.71      | 124.72   |
| 25  | C     | 1054 | BCR  | C28-C27-C26 | -2.64 | 109.34      | 114.06   |
| 25  | D     | 1050 | BCR  | C8-C7-C6    | -2.64 | 119.94      | 127.00   |
| 22  | B     | 1023 | CLA  | O2D-CGD-O1D | -2.64 | 118.71      | 123.85   |
| 25  | c     | 6054 | BCR  | C28-C27-C26 | -2.64 | 109.35      | 114.06   |
| 25  | b     | 6047 | BCR  | C8-C7-C6    | -2.63 | 119.96      | 127.00   |
| 25  | h     | 6049 | BCR  | C28-C27-C26 | -2.63 | 109.36      | 114.06   |
| 25  | d     | 6050 | BCR  | C8-C7-C6    | -2.63 | 119.97      | 127.00   |
| 25  | K     | 1051 | BCR  | C23-C24-C25 | -2.63 | 119.97      | 127.00   |
| 25  | k     | 6051 | BCR  | C23-C24-C25 | -2.63 | 119.98      | 127.00   |
| 25  | k     | 6052 | BCR  | C8-C7-C6    | -2.62 | 119.99      | 127.00   |
| 23  | d     | 6039 | PHO  | O1D-CGD-CBD | -2.62 | 120.74      | 124.72   |
| 25  | C     | 1054 | BCR  | C3-C4-C5    | -2.62 | 109.38      | 114.06   |
| 25  | B     | 1045 | BCR  | C8-C7-C6    | -2.62 | 119.99      | 127.00   |
| 25  | T     | 6048 | BCR  | C3-C4-C5    | -2.62 | 109.38      | 114.06   |
| 25  | h     | 6049 | BCR  | C8-C7-C6    | -2.62 | 119.99      | 127.00   |
| 25  | c     | 6054 | BCR  | C3-C4-C5    | -2.62 | 109.38      | 114.06   |
| 25  | C     | 1052 | BCR  | C8-C7-C6    | -2.62 | 120.00      | 127.00   |
| 25  | H     | 1049 | BCR  | C8-C7-C6    | -2.62 | 120.00      | 127.00   |
| 25  | D     | 1050 | BCR  | C23-C24-C25 | -2.62 | 120.00      | 127.00   |
| 25  | C     | 1054 | BCR  | C8-C7-C6    | -2.62 | 120.00      | 127.00   |
| 25  | b     | 6045 | BCR  | C28-C27-C26 | -2.62 | 109.39      | 114.06   |
| 25  | b     | 6045 | BCR  | C8-C7-C6    | -2.62 | 120.00      | 127.00   |
| 25  | T     | 6048 | BCR  | C8-C7-C6    | -2.62 | 120.00      | 127.00   |
| 25  | B     | 1048 | BCR  | C8-C7-C6    | -2.62 | 120.01      | 127.00   |
| 25  | B     | 1045 | BCR  | C23-C24-C25 | -2.62 | 120.01      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | z     | 6053 | BCR  | C3-C4-C5    | -2.62 | 109.39      | 114.06   |
| 25  | z     | 6053 | BCR  | C8-C7-C6    | -2.62 | 120.01      | 127.00   |
| 25  | B     | 1047 | BCR  | C8-C7-C6    | -2.61 | 120.01      | 127.00   |
| 25  | K     | 1051 | BCR  | C8-C7-C6    | -2.61 | 120.01      | 127.00   |
| 25  | b     | 6045 | BCR  | C23-C24-C25 | -2.61 | 120.01      | 127.00   |
| 25  | B     | 1048 | BCR  | C3-C4-C5    | -2.61 | 109.39      | 114.06   |
| 25  | Z     | 1053 | BCR  | C23-C24-C25 | -2.61 | 120.02      | 127.00   |
| 25  | Z     | 1053 | BCR  | C8-C7-C6    | -2.61 | 120.03      | 127.00   |
| 25  | Z     | 1053 | BCR  | C3-C4-C5    | -2.61 | 109.40      | 114.06   |
| 25  | d     | 6050 | BCR  | C23-C24-C25 | -2.61 | 120.03      | 127.00   |
| 25  | k     | 6051 | BCR  | C8-C7-C6    | -2.61 | 120.03      | 127.00   |
| 25  | T     | 6048 | BCR  | C23-C24-C25 | 2.61  | 133.96      | 127.00   |
| 25  | z     | 6053 | BCR  | C23-C24-C25 | -2.60 | 120.04      | 127.00   |
| 25  | B     | 1048 | BCR  | C23-C24-C25 | 2.60  | 133.94      | 127.00   |
| 25  | c     | 6054 | BCR  | C8-C7-C6    | -2.60 | 120.06      | 127.00   |
| 25  | B     | 1045 | BCR  | C28-C27-C26 | -2.60 | 109.43      | 114.06   |
| 22  | b     | 6011 | CLA  | O2A-CGA-CBA | 2.59  | 119.74      | 111.83   |
| 22  | B     | 1011 | CLA  | O2A-CGA-CBA | 2.59  | 119.74      | 111.83   |
| 25  | k     | 6052 | BCR  | C3-C4-C5    | -2.59 | 109.43      | 114.06   |
| 25  | d     | 6050 | BCR  | C3-C4-C5    | -2.59 | 109.44      | 114.06   |
| 25  | D     | 1050 | BCR  | C3-C4-C5    | -2.59 | 109.44      | 114.06   |
| 24  | a     | 6043 | PQ9  | C6-C5-C4    | 2.59  | 120.57      | 115.28   |
| 25  | B     | 1047 | BCR  | C23-C24-C25 | 2.58  | 133.90      | 127.00   |
| 25  | C     | 1052 | BCR  | C3-C4-C5    | -2.58 | 109.45      | 114.06   |
| 24  | A     | 1043 | PQ9  | C6-C5-C4    | 2.58  | 120.56      | 115.28   |
| 25  | b     | 6047 | BCR  | C3-C4-C5    | -2.58 | 109.46      | 114.06   |
| 25  | d     | 6050 | BCR  | C28-C27-C26 | -2.57 | 109.47      | 114.06   |
| 25  | D     | 1050 | BCR  | C28-C27-C26 | -2.57 | 109.48      | 114.06   |
| 25  | B     | 1047 | BCR  | C3-C4-C5    | -2.57 | 109.48      | 114.06   |
| 25  | b     | 6047 | BCR  | C23-C24-C25 | 2.57  | 133.85      | 127.00   |
| 25  | B     | 1045 | BCR  | C3-C4-C5    | -2.57 | 109.48      | 114.06   |
| 25  | b     | 6045 | BCR  | C3-C4-C5    | -2.56 | 109.49      | 114.06   |
| 25  | h     | 6049 | BCR  | C3-C4-C5    | -2.56 | 109.49      | 114.06   |
| 25  | k     | 6052 | BCR  | C29-C30-C25 | -2.56 | 106.72      | 110.44   |
| 25  | H     | 1049 | BCR  | C3-C4-C5    | -2.56 | 109.50      | 114.06   |
| 25  | k     | 6051 | BCR  | C3-C4-C5    | -2.56 | 109.50      | 114.06   |
| 25  | K     | 1051 | BCR  | C3-C4-C5    | -2.55 | 109.50      | 114.06   |
| 25  | Z     | 1053 | BCR  | C28-C27-C26 | -2.55 | 109.51      | 114.06   |
| 24  | D     | 1042 | PQ9  | C6-C5-C4    | 2.55  | 120.49      | 115.28   |
| 22  | c     | 6030 | CLA  | CAC-C3C-C4C | 2.54  | 128.10      | 124.79   |
| 25  | C     | 1052 | BCR  | C29-C30-C25 | -2.54 | 106.75      | 110.44   |
| 22  | C     | 1030 | CLA  | CAC-C3C-C4C | 2.53  | 128.09      | 124.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | z     | 6053 | BCR  | C28-C27-C26 | -2.53 | 109.54      | 114.06   |
| 24  | d     | 6042 | PQ9  | C6-C5-C4    | 2.53  | 120.46      | 115.28   |
| 22  | d     | 6005 | CLA  | O2D-CGD-O1D | -2.53 | 118.93      | 123.85   |
| 28  | l     | 6061 | MGE  | C2G-O2G-C1B | -2.53 | 111.75      | 117.80   |
| 22  | b     | 6024 | CLA  | O2D-CGD-O1D | -2.52 | 118.94      | 123.85   |
| 28  | L     | 1061 | MGE  | C2G-O2G-C1B | -2.52 | 111.76      | 117.80   |
| 22  | B     | 1024 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | b     | 6018 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | B     | 1009 | CLA  | O2A-CGA-O1A | -2.52 | 117.33      | 123.63   |
| 22  | C     | 1036 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 29  | c     | 6055 | DGD  | C2G-O2G-C1B | -2.51 | 111.78      | 117.80   |
| 22  | C     | 1037 | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 25  | K     | 1051 | BCR  | C28-C27-C26 | -2.51 | 109.57      | 114.06   |
| 22  | B     | 1022 | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 29  | C     | 1057 | DGD  | C2G-O2G-C1B | -2.51 | 111.78      | 117.80   |
| 29  | C     | 1055 | DGD  | C2G-O2G-C1B | -2.51 | 111.78      | 117.80   |
| 29  | B     | 1058 | DGD  | C2G-O2G-C1B | -2.51 | 111.79      | 117.80   |
| 22  | D     | 1005 | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 28  | b     | 6060 | MGE  | C2G-O2G-C1B | -2.51 | 111.79      | 117.80   |
| 22  | C     | 1026 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 22  | C     | 1033 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 26  | a     | 6063 | LHG  | C5-O7-C7    | -2.51 | 111.79      | 117.80   |
| 22  | A     | 1006 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 26  | A     | 1063 | LHG  | C5-O7-C7    | -2.51 | 111.80      | 117.80   |
| 22  | b     | 6022 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 22  | c     | 6035 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 22  | c     | 6033 | CLA  | O2D-CGD-O1D | -2.50 | 118.97      | 123.85   |
| 22  | C     | 1030 | CLA  | O2A-CGA-CBA | 2.50  | 119.47      | 111.83   |
| 22  | C     | 1027 | CLA  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 28  | B     | 1060 | MGE  | C2G-O2G-C1B | -2.50 | 111.81      | 117.80   |
| 22  | B     | 1018 | CLA  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 29  | c     | 6056 | DGD  | C2G-O2G-C1B | -2.50 | 111.81      | 117.80   |
| 29  | c     | 6057 | DGD  | C2G-O2G-C1B | -2.50 | 111.81      | 117.80   |
| 22  | a     | 6006 | CLA  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 25  | k     | 6051 | BCR  | C28-C27-C26 | -2.50 | 109.60      | 114.06   |
| 29  | C     | 1056 | DGD  | C2G-O2G-C1B | -2.50 | 111.82      | 117.80   |
| 22  | c     | 6036 | CLA  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 22  | c     | 6030 | CLA  | O2A-CGA-CBA | 2.50  | 119.45      | 111.83   |
| 22  | K     | 1034 | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 22  | B     | 1016 | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 22  | a     | 6007 | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 22  | c     | 6037 | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6019 | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 29  | b     | 6058 | DGD  | C2G-O2G-C1B | -2.49 | 111.83      | 117.80   |
| 22  | b     | 6009 | CLA  | O2A-CGA-O1A | -2.49 | 117.39      | 123.63   |
| 22  | C     | 1032 | CLA  | O2D-CGD-O1D | -2.49 | 118.99      | 123.85   |
| 22  | a     | 6003 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 22  | A     | 1003 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 22  | b     | 6020 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 28  | D     | 1059 | MGE  | C2G-O2G-C1B | -2.49 | 111.84      | 117.80   |
| 22  | B     | 1012 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 22  | B     | 1019 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 22  | c     | 6026 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 22  | b     | 6012 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 28  | d     | 6062 | MGE  | C2G-O2G-C1B | -2.49 | 111.85      | 117.80   |
| 22  | B     | 1020 | CLA  | O2D-CGD-O1D | -2.48 | 119.01      | 123.85   |
| 22  | k     | 6034 | CLA  | O2D-CGD-O1D | -2.48 | 119.01      | 123.85   |
| 22  | C     | 1025 | CLA  | O2D-CGD-O1D | -2.48 | 119.01      | 123.85   |
| 22  | C     | 1035 | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 28  | D     | 1062 | MGE  | C2G-O2G-C1B | -2.48 | 111.86      | 117.80   |
| 22  | c     | 6025 | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 22  | A     | 1007 | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 28  | d     | 6059 | MGE  | C2G-O2G-C1B | -2.48 | 111.86      | 117.80   |
| 22  | b     | 6011 | CLA  | O2A-CGA-O1A | -2.48 | 117.43      | 123.63   |
| 22  | c     | 6031 | CLA  | O2D-CGD-O1D | -2.48 | 119.03      | 123.85   |
| 22  | c     | 6032 | CLA  | O2D-CGD-O1D | -2.48 | 119.03      | 123.85   |
| 22  | D     | 1004 | CLA  | O2D-CGD-O1D | -2.48 | 119.03      | 123.85   |
| 22  | b     | 6016 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | c     | 6027 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | B     | 1015 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | B     | 1014 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | C     | 1031 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 22  | b     | 6014 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 22  | B     | 1013 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 22  | b     | 6013 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 22  | H     | 1017 | CLA  | O2D-CGD-O1D | -2.47 | 119.05      | 123.85   |
| 22  | d     | 6004 | CLA  | O2D-CGD-O1D | -2.47 | 119.05      | 123.85   |
| 22  | h     | 6017 | CLA  | O2D-CGD-O1D | -2.47 | 119.05      | 123.85   |
| 22  | b     | 6015 | CLA  | O2D-CGD-O1D | -2.46 | 119.05      | 123.85   |
| 22  | B     | 1011 | CLA  | O2A-CGA-O1A | -2.46 | 117.48      | 123.63   |
| 22  | D     | 1008 | CLA  | CMC-C2C-C1C | 2.45  | 128.85      | 125.03   |
| 22  | d     | 6008 | CLA  | CMC-C2C-C1C | 2.44  | 128.85      | 125.03   |
| 22  | b     | 6009 | CLA  | CHC-C1C-C2C | -2.44 | 120.01      | 126.95   |
| 22  | C     | 1028 | CLA  | O2D-CGD-O1D | -2.44 | 119.10      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1009 | CLA  | CHC-C1C-C2C | -2.44 | 120.03      | 126.95   |
| 23  | A     | 1038 | PHO  | O2D-CGD-O1D | -2.43 | 119.11      | 123.85   |
| 23  | D     | 1039 | PHO  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 23  | a     | 6038 | PHO  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 22  | c     | 6028 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 22  | b     | 6023 | CLA  | CMC-C2C-C1C | 2.41  | 128.81      | 125.03   |
| 22  | b     | 6021 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 22  | C     | 1030 | CLA  | CMC-C2C-C1C | 2.41  | 128.80      | 125.03   |
| 22  | B     | 1023 | CLA  | CMC-C2C-C1C | 2.41  | 128.80      | 125.03   |
| 23  | d     | 6039 | PHO  | O2D-CGD-O1D | -2.41 | 119.16      | 123.85   |
| 22  | B     | 1021 | CLA  | O2D-CGD-O1D | -2.41 | 119.16      | 123.85   |
| 22  | c     | 6030 | CLA  | CMC-C2C-C1C | 2.41  | 128.79      | 125.03   |
| 25  | h     | 6049 | BCR  | C23-C24-C25 | -2.40 | 120.58      | 127.00   |
| 23  | d     | 6039 | PHO  | CMA-C3A-C4A | -2.40 | 109.44      | 114.61   |
| 25  | H     | 1049 | BCR  | C23-C24-C25 | -2.40 | 120.59      | 127.00   |
| 25  | t     | 1046 | BCR  | C28-C27-C26 | -2.40 | 109.78      | 114.06   |
| 22  | B     | 1021 | CLA  | O2A-CGA-CBA | 2.40  | 119.14      | 111.83   |
| 23  | D     | 1039 | PHO  | CMA-C3A-C4A | -2.39 | 109.45      | 114.61   |
| 22  | B     | 1021 | CLA  | CMC-C2C-C1C | 2.39  | 128.77      | 125.03   |
| 25  | T     | 6046 | BCR  | C28-C27-C26 | -2.39 | 109.80      | 114.06   |
| 22  | b     | 6021 | CLA  | O2A-CGA-CBA | 2.38  | 119.11      | 111.83   |
| 22  | B     | 1010 | CLA  | CMC-C2C-C1C | 2.38  | 128.75      | 125.03   |
| 25  | c     | 6054 | BCR  | C23-C24-C25 | -2.38 | 120.64      | 127.00   |
| 25  | C     | 1054 | BCR  | C23-C24-C25 | -2.38 | 120.64      | 127.00   |
| 22  | b     | 6010 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 24  | A     | 1043 | PQ9  | C45-C43-C44 | 2.37  | 120.05      | 114.59   |
| 24  | a     | 6043 | PQ9  | C45-C43-C44 | 2.37  | 120.05      | 114.59   |
| 22  | b     | 6021 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 22  | b     | 6018 | CLA  | CMC-C2C-C1C | 2.37  | 128.73      | 125.03   |
| 23  | A     | 1038 | PHO  | CMA-C3A-C4A | -2.37 | 109.51      | 114.61   |
| 22  | C     | 1029 | CLA  | CMC-C2C-C1C | 2.36  | 128.72      | 125.03   |
| 23  | a     | 6038 | PHO  | CMA-C3A-C4A | -2.36 | 109.53      | 114.61   |
| 22  | B     | 1021 | CLA  | O2A-CGA-O1A | -2.36 | 117.73      | 123.63   |
| 22  | k     | 6034 | CLA  | CMC-C2C-C1C | 2.36  | 128.72      | 125.03   |
| 24  | d     | 6042 | PQ9  | C45-C43-C44 | 2.35  | 120.00      | 114.59   |
| 22  | b     | 6014 | CLA  | CMC-C2C-C1C | 2.35  | 128.71      | 125.03   |
| 24  | D     | 1042 | PQ9  | C45-C43-C44 | 2.35  | 120.00      | 114.59   |
| 22  | D     | 1004 | CLA  | CMC-C2C-C1C | 2.35  | 128.70      | 125.03   |
| 22  | K     | 1034 | CLA  | CMC-C2C-C1C | 2.35  | 128.70      | 125.03   |
| 25  | T     | 6046 | BCR  | C23-C24-C25 | -2.35 | 120.73      | 127.00   |
| 22  | C     | 1037 | CLA  | CMC-C2C-C1C | 2.35  | 128.70      | 125.03   |
| 22  | b     | 6021 | CLA  | O2A-CGA-O1A | -2.35 | 117.76      | 123.63   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | d     | 6008 | CLA  | CHC-C1C-C2C | -2.34 | 120.29      | 126.95   |
| 25  | t     | 1046 | BCR  | C23-C24-C25 | -2.34 | 120.74      | 127.00   |
| 22  | B     | 1012 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 22  | a     | 6006 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 22  | b     | 6023 | CLA  | CHC-C1C-C2C | -2.34 | 120.30      | 126.95   |
| 22  | c     | 6029 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 22  | D     | 1008 | CLA  | CHC-C1C-C2C | -2.34 | 120.30      | 126.95   |
| 22  | c     | 6026 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 22  | B     | 1018 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 31  | V     | 1041 | HEM  | C3B-C2B-C1B | 2.34  | 108.17      | 106.41   |
| 22  | c     | 6031 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 22  | d     | 6004 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 22  | C     | 1026 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 22  | A     | 1007 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 22  | b     | 6012 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 22  | c     | 6033 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 22  | B     | 1021 | CLA  | CHC-C1C-C2C | -2.33 | 120.31      | 126.95   |
| 22  | B     | 1014 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 22  | b     | 6024 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 22  | c     | 6027 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 22  | B     | 1023 | CLA  | CHC-C1C-C2C | -2.33 | 120.32      | 126.95   |
| 22  | c     | 6037 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 22  | k     | 6034 | CLA  | CHC-C1C-C2C | -2.33 | 120.33      | 126.95   |
| 31  | v     | 6041 | HEM  | C1B-NB-C4B  | 2.33  | 107.97      | 105.21   |
| 22  | b     | 6022 | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 22  | b     | 6021 | CLA  | CHC-C1C-C2C | -2.33 | 120.33      | 126.95   |
| 22  | B     | 1016 | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 22  | B     | 1010 | CLA  | CHC-C1C-C2C | -2.33 | 120.34      | 126.95   |
| 22  | b     | 6010 | CLA  | CHC-C1C-C2C | -2.33 | 120.34      | 126.95   |
| 22  | a     | 6007 | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 22  | c     | 6032 | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 22  | B     | 1009 | CLA  | O1D-CGD-CBD | -2.32 | 119.93      | 124.52   |
| 22  | C     | 1033 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | D     | 1005 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | B     | 1022 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | C     | 1032 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | b     | 6020 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | C     | 1029 | CLA  | CHC-C1C-C2C | -2.32 | 120.35      | 126.95   |
| 22  | C     | 1025 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | C     | 1035 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | a     | 6003 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 22  | c     | 6027 | CLA  | CHC-C1C-C2C | -2.32 | 120.36      | 126.95   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | a     | 6007 | CLA  | CHC-C1C-C2C | -2.32 | 120.36      | 126.95   |
| 22  | H     | 1017 | CLA  | CMC-C2C-C1C | 2.32  | 128.65      | 125.03   |
| 22  | c     | 6035 | CLA  | CMC-C2C-C1C | 2.32  | 128.65      | 125.03   |
| 22  | B     | 1024 | CLA  | CMC-C2C-C1C | 2.32  | 128.65      | 125.03   |
| 22  | d     | 6005 | CLA  | CMC-C2C-C1C | 2.32  | 128.65      | 125.03   |
| 22  | A     | 1003 | CLA  | CMC-C2C-C1C | 2.32  | 128.65      | 125.03   |
| 22  | b     | 6012 | CLA  | CHC-C1C-C2C | -2.31 | 120.37      | 126.95   |
| 22  | h     | 6017 | CLA  | CMC-C2C-C1C | 2.31  | 128.65      | 125.03   |
| 22  | B     | 1022 | CLA  | CHC-C1C-C2C | -2.31 | 120.37      | 126.95   |
| 22  | B     | 1020 | CLA  | CMC-C2C-C1C | 2.31  | 128.65      | 125.03   |
| 22  | B     | 1012 | CLA  | CHC-C1C-C2C | -2.31 | 120.38      | 126.95   |
| 22  | K     | 1034 | CLA  | CHC-C1C-C2C | -2.31 | 120.38      | 126.95   |
| 22  | b     | 6022 | CLA  | CHC-C1C-C2C | -2.31 | 120.38      | 126.95   |
| 22  | c     | 6031 | CLA  | CHC-C1C-C2C | -2.31 | 120.38      | 126.95   |
| 22  | A     | 1006 | CLA  | CMC-C2C-C1C | 2.31  | 128.65      | 125.03   |
| 22  | c     | 6028 | CLA  | CMC-C2C-C1C | 2.31  | 128.65      | 125.03   |
| 22  | C     | 1033 | CLA  | CHC-C1C-C2C | -2.31 | 120.38      | 126.95   |
| 22  | a     | 6003 | CLA  | CHC-C1C-C2C | -2.31 | 120.38      | 126.95   |
| 22  | c     | 6033 | CLA  | CHC-C1C-C2C | -2.31 | 120.38      | 126.95   |
| 22  | A     | 1007 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | B     | 1011 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | B     | 1013 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | C     | 1028 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | C     | 1027 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | b     | 6018 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | b     | 6011 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | B     | 1019 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | b     | 6020 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | c     | 6029 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | C     | 1027 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | C     | 1036 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | b     | 6019 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | c     | 6036 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | B     | 1014 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | a     | 6006 | CLA  | CHC-C1C-C2C | -2.31 | 120.39      | 126.95   |
| 22  | b     | 6013 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | C     | 1026 | CLA  | CHC-C1C-C2C | -2.31 | 120.40      | 126.95   |
| 22  | b     | 6019 | CLA  | CHC-C1C-C2C | -2.31 | 120.40      | 126.95   |
| 22  | c     | 6025 | CLA  | CHC-C1C-C2C | -2.31 | 120.40      | 126.95   |
| 22  | b     | 6016 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 22  | B     | 1023 | CLA  | O2A-CGA-CBA | 2.30  | 118.86      | 111.83   |
| 31  | v     | 6041 | HEM  | C3B-C2B-C1B | 2.30  | 108.14      | 106.41   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6014 | CLA  | CHC-C1C-C2C | -2.30 | 120.40      | 126.95   |
| 22  | C     | 1025 | CLA  | CHC-C1C-C2C | -2.30 | 120.40      | 126.95   |
| 22  | c     | 6026 | CLA  | CHC-C1C-C2C | -2.30 | 120.40      | 126.95   |
| 22  | d     | 6005 | CLA  | CHC-C1C-C2C | -2.30 | 120.40      | 126.95   |
| 22  | b     | 6009 | CLA  | O1D-CGD-CBD | -2.30 | 119.98      | 124.52   |
| 22  | c     | 6036 | CLA  | CHC-C1C-C2C | -2.30 | 120.41      | 126.95   |
| 22  | B     | 1020 | CLA  | CHC-C1C-C2C | -2.30 | 120.41      | 126.95   |
| 22  | D     | 1005 | CLA  | CHC-C1C-C2C | -2.30 | 120.41      | 126.95   |
| 22  | b     | 6024 | CLA  | CHC-C1C-C2C | -2.30 | 120.41      | 126.95   |
| 22  | C     | 1031 | CLA  | CMC-C2C-C1C | 2.30  | 128.63      | 125.03   |
| 22  | A     | 1003 | CLA  | CHC-C1C-C2C | -2.30 | 120.41      | 126.95   |
| 22  | B     | 1016 | CLA  | CHC-C1C-C2C | -2.30 | 120.41      | 126.95   |
| 22  | b     | 6015 | CLA  | CMC-C2C-C1C | 2.30  | 128.63      | 125.03   |
| 22  | C     | 1031 | CLA  | CHC-C1C-C2C | -2.30 | 120.41      | 126.95   |
| 31  | V     | 1041 | HEM  | C1B-NB-C4B  | 2.30  | 107.93      | 105.21   |
| 22  | B     | 1018 | CLA  | CHC-C1C-C2C | -2.30 | 120.42      | 126.95   |
| 22  | b     | 6013 | CLA  | CHC-C1C-C2C | -2.30 | 120.42      | 126.95   |
| 22  | B     | 1013 | CLA  | CHC-C1C-C2C | -2.30 | 120.42      | 126.95   |
| 22  | b     | 6023 | CLA  | O2A-CGA-CBA | 2.30  | 118.84      | 111.83   |
| 22  | C     | 1036 | CLA  | CHC-C1C-C2C | -2.30 | 120.42      | 126.95   |
| 22  | c     | 6025 | CLA  | CMC-C2C-C1C | 2.30  | 128.62      | 125.03   |
| 22  | b     | 6015 | CLA  | CHC-C1C-C2C | -2.30 | 120.42      | 126.95   |
| 31  | F     | 1040 | HEM  | C1B-NB-C4B  | 2.30  | 107.92      | 105.21   |
| 22  | C     | 1032 | CLA  | CHC-C1C-C2C | -2.29 | 120.43      | 126.95   |
| 22  | B     | 1019 | CLA  | CHC-C1C-C2C | -2.29 | 120.43      | 126.95   |
| 22  | A     | 1006 | CLA  | CHC-C1C-C2C | -2.29 | 120.43      | 126.95   |
| 22  | D     | 1004 | CLA  | CHC-C1C-C2C | -2.29 | 120.43      | 126.95   |
| 22  | H     | 1017 | CLA  | CHC-C1C-C2C | -2.29 | 120.43      | 126.95   |
| 22  | C     | 1035 | CLA  | CHC-C1C-C2C | -2.29 | 120.44      | 126.95   |
| 22  | c     | 6032 | CLA  | CHC-C1C-C2C | -2.29 | 120.44      | 126.95   |
| 22  | c     | 6028 | CLA  | CHC-C1C-C2C | -2.29 | 120.44      | 126.95   |
| 22  | C     | 1028 | CLA  | CHC-C1C-C2C | -2.29 | 120.44      | 126.95   |
| 22  | B     | 1024 | CLA  | CHC-C1C-C2C | -2.29 | 120.45      | 126.95   |
| 22  | h     | 6017 | CLA  | CHC-C1C-C2C | -2.29 | 120.45      | 126.95   |
| 22  | B     | 1015 | CLA  | CHC-C1C-C2C | -2.29 | 120.45      | 126.95   |
| 22  | B     | 1015 | CLA  | CMC-C2C-C1C | 2.28  | 128.60      | 125.03   |
| 22  | b     | 6010 | CLA  | CHB-C1B-NB  | -2.28 | 120.63      | 124.05   |
| 22  | b     | 6016 | CLA  | CHC-C1C-C2C | -2.28 | 120.46      | 126.95   |
| 31  | f     | 6040 | HEM  | C1B-NB-C4B  | 2.28  | 107.91      | 105.21   |
| 22  | c     | 6035 | CLA  | CHC-C1C-C2C | -2.28 | 120.47      | 126.95   |
| 22  | d     | 6004 | CLA  | CHC-C1C-C2C | -2.28 | 120.47      | 126.95   |
| 22  | B     | 1010 | CLA  | CHB-C1B-NB  | -2.28 | 120.63      | 124.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | b     | 6009 | CLA  | CMC-C2C-C1C | 2.27  | 128.59      | 125.03   |
| 22  | c     | 6037 | CLA  | CHC-C1C-C2C | -2.27 | 120.49      | 126.95   |
| 22  | C     | 1030 | CLA  | O1D-CGD-CBD | -2.27 | 120.04      | 124.52   |
| 22  | c     | 6030 | CLA  | O1D-CGD-CBD | -2.27 | 120.04      | 124.52   |
| 31  | F     | 1040 | HEM  | C3B-C2B-C1B | 2.27  | 108.11      | 106.41   |
| 22  | C     | 1037 | CLA  | CHC-C1C-C2C | -2.27 | 120.50      | 126.95   |
| 22  | C     | 1030 | CLA  | CHC-C1C-C2C | -2.26 | 120.52      | 126.95   |
| 31  | f     | 6040 | HEM  | C3B-C2B-C1B | 2.26  | 108.11      | 106.41   |
| 22  | B     | 1009 | CLA  | CMC-C2C-C1C | 2.25  | 128.56      | 125.03   |
| 31  | v     | 6041 | HEM  | C3B-C4B-NB  | -2.25 | 107.85      | 109.47   |
| 22  | c     | 6030 | CLA  | CHC-C1C-C2C | -2.25 | 120.55      | 126.95   |
| 22  | b     | 6011 | CLA  | CMC-C2C-C1C | 2.24  | 128.53      | 125.03   |
| 22  | B     | 1011 | CLA  | CMC-C2C-C1C | 2.23  | 128.52      | 125.03   |
| 25  | A     | 1044 | BCR  | C1-C6-C5    | -2.23 | 119.59      | 122.64   |
| 25  | b     | 6047 | BCR  | C24-C25-C26 | -2.22 | 116.43      | 121.56   |
| 22  | C     | 1030 | CLA  | O2A-CGA-O1A | -2.22 | 118.07      | 123.63   |
| 31  | V     | 1041 | HEM  | C3B-C4B-NB  | -2.21 | 107.88      | 109.47   |
| 25  | a     | 6044 | BCR  | C1-C6-C5    | -2.21 | 119.61      | 122.64   |
| 25  | B     | 1047 | BCR  | C24-C25-C26 | -2.21 | 116.46      | 121.56   |
| 22  | B     | 1010 | CLA  | O1D-CGD-CBD | -2.20 | 120.17      | 124.52   |
| 22  | c     | 6030 | CLA  | O2A-CGA-O1A | -2.20 | 118.12      | 123.63   |
| 22  | b     | 6010 | CLA  | O1D-CGD-CBD | -2.20 | 120.19      | 124.52   |
| 25  | T     | 6048 | BCR  | C24-C25-C26 | -2.19 | 116.51      | 121.56   |
| 22  | b     | 6023 | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 22  | B     | 1023 | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 25  | t     | 1046 | BCR  | C8-C7-C6    | -2.18 | 121.16      | 127.00   |
| 25  | B     | 1048 | BCR  | C24-C25-C26 | -2.18 | 116.53      | 121.56   |
| 22  | c     | 6029 | CLA  | O2A-CGA-O1A | -2.18 | 118.17      | 123.63   |
| 31  | F     | 1040 | HEM  | C3B-C4B-NB  | -2.18 | 107.90      | 109.47   |
| 22  | C     | 1029 | CLA  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |
| 22  | D     | 1008 | CLA  | CHB-C1B-NB  | -2.17 | 120.80      | 124.05   |
| 25  | T     | 6046 | BCR  | C8-C7-C6    | -2.16 | 121.23      | 127.00   |
| 25  | a     | 6044 | BCR  | C27-C26-C25 | -2.16 | 119.79      | 122.70   |
| 24  | d     | 6042 | PQ9  | C41-C42-C43 | -2.16 | 120.45      | 127.64   |
| 22  | B     | 1023 | CLA  | O1D-CGD-CBD | -2.15 | 120.27      | 124.52   |
| 22  | d     | 6008 | CLA  | CHB-C1B-NB  | -2.15 | 120.82      | 124.05   |
| 22  | b     | 6021 | CLA  | O1D-CGD-CBD | -2.15 | 120.28      | 124.52   |
| 25  | A     | 1044 | BCR  | C27-C26-C25 | -2.15 | 119.80      | 122.70   |
| 22  | b     | 6009 | CLA  | CHB-C1B-NB  | -2.15 | 120.83      | 124.05   |
| 22  | b     | 6023 | CLA  | O1D-CGD-CBD | -2.14 | 120.29      | 124.52   |
| 24  | A     | 1043 | PQ9  | C41-C42-C43 | -2.14 | 120.49      | 127.64   |
| 24  | a     | 6043 | PQ9  | C41-C42-C43 | -2.14 | 120.50      | 127.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | D     | 1042 | PQ9  | C41-C42-C43 | -2.14 | 120.50      | 127.64   |
| 31  | f     | 6040 | HEM  | C3B-C4B-NB  | -2.14 | 107.93      | 109.47   |
| 25  | T     | 6046 | BCR  | C2-C1-C6    | -2.14 | 107.33      | 110.44   |
| 22  | B     | 1021 | CLA  | O1D-CGD-CBD | -2.14 | 120.30      | 124.52   |
| 25  | a     | 6044 | BCR  | C29-C30-C25 | -2.14 | 107.34      | 110.44   |
| 22  | B     | 1009 | CLA  | O2A-CGA-CBA | 2.13  | 118.33      | 111.83   |
| 25  | a     | 6044 | BCR  | C4-C5-C6    | -2.13 | 119.83      | 122.70   |
| 25  | C     | 1052 | BCR  | C24-C25-C26 | 2.13  | 126.45      | 121.56   |
| 22  | b     | 6009 | CLA  | O2A-CGA-CBA | 2.13  | 118.32      | 111.83   |
| 31  | v     | 6041 | HEM  | C2A-C1A-NA  | -2.12 | 107.80      | 110.15   |
| 22  | c     | 6030 | CLA  | CHB-C1B-NB  | -2.12 | 120.86      | 124.05   |
| 25  | t     | 1046 | BCR  | C2-C1-C6    | -2.12 | 107.36      | 110.44   |
| 25  | A     | 1044 | BCR  | C29-C30-C25 | -2.12 | 107.36      | 110.44   |
| 22  | C     | 1030 | CLA  | CHB-C1B-NB  | -2.12 | 120.87      | 124.05   |
| 25  | A     | 1044 | BCR  | C4-C5-C6    | -2.12 | 119.84      | 122.70   |
| 25  | T     | 6048 | BCR  | C27-C26-C25 | -2.11 | 119.85      | 122.70   |
| 22  | c     | 6037 | CLA  | CHB-C1B-NB  | -2.11 | 120.89      | 124.05   |
| 25  | k     | 6052 | BCR  | C24-C25-C26 | 2.11  | 126.41      | 121.56   |
| 22  | C     | 1037 | CLA  | CHB-C1B-NB  | -2.10 | 120.90      | 124.05   |
| 22  | c     | 6037 | CLA  | O1D-CGD-CBD | -2.10 | 120.38      | 124.52   |
| 22  | b     | 6014 | CLA  | CHB-C1B-NB  | -2.10 | 120.91      | 124.05   |
| 22  | B     | 1009 | CLA  | CHB-C1B-NB  | -2.09 | 120.91      | 124.05   |
| 22  | c     | 6032 | CLA  | CHB-C1B-NB  | -2.09 | 120.91      | 124.05   |
| 25  | t     | 1046 | BCR  | C36-C18-C17 | -2.09 | 119.43      | 122.82   |
| 22  | C     | 1037 | CLA  | O1D-CGD-CBD | -2.09 | 120.40      | 124.52   |
| 31  | F     | 1040 | HEM  | C2A-C1A-NA  | -2.09 | 107.83      | 110.15   |
| 22  | a     | 6006 | CLA  | O1D-CGD-CBD | -2.09 | 120.40      | 124.52   |
| 22  | C     | 1035 | CLA  | CHB-C1B-NB  | -2.08 | 120.92      | 124.05   |
| 22  | d     | 6004 | CLA  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 22  | b     | 6024 | CLA  | CHB-C1B-NB  | -2.08 | 120.92      | 124.05   |
| 22  | A     | 1006 | CLA  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 22  | b     | 6019 | CLA  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 22  | k     | 6034 | CLA  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 22  | a     | 6006 | CLA  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 22  | A     | 1006 | CLA  | O1D-CGD-CBD | -2.08 | 120.42      | 124.52   |
| 31  | V     | 1041 | HEM  | C2A-C1A-NA  | -2.08 | 107.85      | 110.15   |
| 22  | B     | 1019 | CLA  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 22  | c     | 6035 | CLA  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 22  | B     | 1020 | CLA  | CHB-C1B-NB  | -2.08 | 120.94      | 124.05   |
| 22  | c     | 6035 | CLA  | O1D-CGD-CBD | -2.08 | 120.42      | 124.52   |
| 22  | K     | 1034 | CLA  | CHB-C1B-NB  | -2.08 | 120.94      | 124.05   |
| 22  | b     | 6020 | CLA  | CHB-C1B-NB  | -2.08 | 120.94      | 124.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 1032 | CLA  | CHB-C1B-NB  | -2.07 | 120.94      | 124.05   |
| 22  | a     | 6007 | CLA  | CHB-C1B-NB  | -2.07 | 120.94      | 124.05   |
| 22  | k     | 6034 | CLA  | O1D-CGD-CBD | -2.07 | 120.43      | 124.52   |
| 22  | C     | 1035 | CLA  | O1D-CGD-CBD | -2.07 | 120.43      | 124.52   |
| 25  | T     | 6046 | BCR  | C36-C18-C17 | -2.07 | 119.46      | 122.82   |
| 22  | K     | 1034 | CLA  | O1D-CGD-CBD | -2.07 | 120.43      | 124.52   |
| 25  | B     | 1048 | BCR  | C27-C26-C25 | -2.07 | 119.91      | 122.70   |
| 22  | B     | 1014 | CLA  | CHB-C1B-NB  | -2.07 | 120.95      | 124.05   |
| 22  | b     | 6018 | CLA  | CHB-C1B-NB  | -2.07 | 120.95      | 124.05   |
| 22  | D     | 1004 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 22  | c     | 6026 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 22  | B     | 1018 | CLA  | CHB-C1B-NB  | -2.07 | 120.95      | 124.05   |
| 22  | B     | 1024 | CLA  | CHB-C1B-NB  | -2.07 | 120.95      | 124.05   |
| 22  | b     | 6021 | CLA  | CHB-C1B-NB  | -2.06 | 120.95      | 124.05   |
| 22  | B     | 1021 | CLA  | CHB-C1B-NB  | -2.06 | 120.95      | 124.05   |
| 31  | f     | 6040 | HEM  | C2A-C1A-NA  | -2.06 | 107.86      | 110.15   |
| 22  | c     | 6027 | CLA  | O1D-CGD-CBD | -2.06 | 120.45      | 124.52   |
| 22  | b     | 6020 | CLA  | O1D-CGD-CBD | -2.06 | 120.45      | 124.52   |
| 22  | c     | 6027 | CLA  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 25  | T     | 6046 | BCR  | C27-C26-C25 | -2.06 | 119.92      | 122.70   |
| 22  | C     | 1031 | CLA  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 22  | B     | 1022 | CLA  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 22  | b     | 6016 | CLA  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 22  | b     | 6021 | CLA  | CAA-CBA-CGA | -2.06 | 107.37      | 113.21   |
| 22  | d     | 6008 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 22  | H     | 1017 | CLA  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 22  | C     | 1027 | CLA  | O1D-CGD-CBD | -2.06 | 120.46      | 124.52   |
| 22  | B     | 1013 | CLA  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 22  | C     | 1027 | CLA  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 22  | D     | 1008 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 25  | t     | 1046 | BCR  | C27-C26-C25 | -2.06 | 119.93      | 122.70   |
| 22  | C     | 1026 | CLA  | CHB-C1B-NB  | -2.06 | 120.97      | 124.05   |
| 22  | c     | 6031 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | B     | 1016 | CLA  | CHB-C1B-NB  | -2.05 | 120.97      | 124.05   |
| 22  | B     | 1022 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | b     | 6022 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | B     | 1020 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | B     | 1018 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | C     | 1026 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | c     | 6036 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | B     | 1015 | CLA  | CHB-C1B-NB  | -2.05 | 120.97      | 124.05   |
| 22  | h     | 6017 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | h     | 6017 | CLA  | CHB-C1B-NB  | -2.05 | 120.97      | 124.05   |
| 25  | A     | 1044 | BCR  | C8-C7-C6    | -2.05 | 121.52      | 127.00   |
| 25  | b     | 6047 | BCR  | C27-C26-C25 | -2.05 | 119.93      | 122.70   |
| 22  | b     | 6013 | CLA  | CHB-C1B-NB  | -2.05 | 120.97      | 124.05   |
| 22  | D     | 1005 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | C     | 1036 | CLA  | CHB-C1B-NB  | -2.05 | 120.97      | 124.05   |
| 22  | B     | 1014 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 25  | T     | 6046 | BCR  | C1-C6-C7    | 2.05  | 121.20      | 115.65   |
| 22  | b     | 6018 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 25  | a     | 6044 | BCR  | C8-C7-C6    | -2.05 | 121.53      | 127.00   |
| 22  | b     | 6016 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | c     | 6025 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | B     | 1016 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | H     | 1017 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | a     | 6007 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | A     | 1007 | CLA  | CHB-C1B-NB  | -2.05 | 120.98      | 124.05   |
| 22  | C     | 1025 | CLA  | CHB-C1B-NB  | -2.05 | 120.98      | 124.05   |
| 22  | b     | 6015 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | C     | 1032 | CLA  | O1D-CGD-CBD | -2.04 | 120.48      | 124.52   |
| 22  | B     | 1013 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 22  | b     | 6013 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 25  | B     | 1047 | BCR  | C27-C26-C25 | -2.04 | 119.94      | 122.70   |
| 22  | a     | 6003 | CLA  | CHB-C1B-NB  | -2.04 | 120.98      | 124.05   |
| 22  | B     | 1021 | CLA  | CAA-CBA-CGA | -2.04 | 107.41      | 113.21   |
| 22  | C     | 1033 | CLA  | CHB-C1B-NB  | -2.04 | 120.98      | 124.05   |
| 22  | b     | 6015 | CLA  | CHB-C1B-NB  | -2.04 | 120.98      | 124.05   |
| 22  | b     | 6022 | CLA  | CHB-C1B-NB  | -2.04 | 120.98      | 124.05   |
| 22  | c     | 6029 | CLA  | CHB-C1B-NB  | -2.04 | 120.98      | 124.05   |
| 22  | c     | 6036 | CLA  | CHB-C1B-NB  | -2.04 | 120.98      | 124.05   |
| 22  | B     | 1012 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 25  | c     | 6054 | BCR  | C4-C5-C6    | -2.04 | 119.94      | 122.70   |
| 22  | A     | 1007 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 25  | t     | 1046 | BCR  | C1-C6-C7    | 2.04  | 121.19      | 115.65   |
| 22  | C     | 1029 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 22  | B     | 1024 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 22  | c     | 6032 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 22  | d     | 6005 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 25  | Z     | 1053 | BCR  | C4-C5-C6    | -2.04 | 119.95      | 122.70   |
| 22  | c     | 6031 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 22  | A     | 1003 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 22  | c     | 6028 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 25  | C     | 1054 | BCR  | C4-C5-C6    | -2.04 | 119.95      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | D     | 1005 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 22  | D     | 1004 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 22  | d     | 6004 | CLA  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 22  | b     | 6014 | CLA  | O1D-CGD-CBD | -2.04 | 120.50      | 124.52   |
| 22  | b     | 6023 | CLA  | CHB-C1B-NB  | -2.04 | 121.00      | 124.05   |
| 25  | b     | 6047 | BCR  | C4-C5-C6    | -2.04 | 119.95      | 122.70   |
| 22  | C     | 1028 | CLA  | CHB-C1B-NB  | -2.03 | 121.00      | 124.05   |
| 25  | z     | 6053 | BCR  | C27-C26-C25 | -2.03 | 119.95      | 122.70   |
| 25  | z     | 6053 | BCR  | C4-C5-C6    | -2.03 | 119.96      | 122.70   |
| 22  | C     | 1036 | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | d     | 6005 | CLA  | CHB-C1B-NB  | -2.03 | 121.00      | 124.05   |
| 22  | C     | 1025 | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | c     | 6026 | CLA  | CHB-C1B-NB  | -2.03 | 121.00      | 124.05   |
| 22  | B     | 1019 | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | C     | 1031 | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 25  | B     | 1048 | BCR  | C4-C5-C6    | -2.03 | 119.96      | 122.70   |
| 22  | b     | 6011 | CLA  | CED-O2D-CGD | 2.03  | 120.52      | 115.92   |
| 22  | b     | 6012 | CLA  | CHB-C1B-NB  | -2.03 | 121.00      | 124.05   |
| 22  | c     | 6033 | CLA  | CHB-C1B-NB  | -2.03 | 121.00      | 124.05   |
| 22  | b     | 6019 | CLA  | O1D-CGD-CBD | -2.03 | 120.52      | 124.52   |
| 22  | B     | 1015 | CLA  | O1D-CGD-CBD | -2.03 | 120.52      | 124.52   |
| 22  | B     | 1023 | CLA  | CHB-C1B-NB  | -2.03 | 121.01      | 124.05   |
| 22  | b     | 6010 | CLA  | O2A-CGA-O1A | -2.02 | 118.56      | 123.63   |
| 22  | b     | 6024 | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 22  | B     | 1011 | CLA  | CED-O2D-CGD | 2.02  | 120.50      | 115.92   |
| 25  | T     | 6048 | BCR  | C4-C5-C6    | -2.02 | 119.97      | 122.70   |
| 22  | A     | 1003 | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 25  | d     | 6050 | BCR  | C4-C5-C6    | -2.02 | 119.98      | 122.70   |
| 22  | C     | 1033 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 25  | D     | 1050 | BCR  | C4-C5-C6    | -2.02 | 119.98      | 122.70   |
| 22  | B     | 1012 | CLA  | O1D-CGD-CBD | -2.01 | 120.55      | 124.52   |
| 22  | c     | 6028 | CLA  | O1D-CGD-CBD | -2.01 | 120.55      | 124.52   |
| 22  | B     | 1010 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 25  | B     | 1045 | BCR  | C27-C26-C25 | -2.01 | 119.99      | 122.70   |
| 22  | b     | 6011 | CLA  | CHB-C1B-NB  | -2.01 | 121.03      | 124.05   |
| 22  | c     | 6025 | CLA  | CHB-C1B-NB  | -2.01 | 121.03      | 124.05   |
| 22  | c     | 6033 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 22  | B     | 1011 | CLA  | CHB-C1B-NB  | -2.01 | 121.04      | 124.05   |
| 22  | a     | 6003 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 22  | b     | 6012 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 25  | D     | 1050 | BCR  | C27-C26-C25 | -2.00 | 120.00      | 122.70   |

All (162) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | A     | 1003 | CLA  | C8   |
| 22  | A     | 1003 | CLA  | ND   |
| 22  | A     | 1006 | CLA  | C8   |
| 22  | A     | 1006 | CLA  | ND   |
| 22  | A     | 1007 | CLA  | ND   |
| 22  | B     | 1009 | CLA  | CBD  |
| 22  | B     | 1009 | CLA  | ND   |
| 22  | B     | 1010 | CLA  | C8   |
| 22  | B     | 1010 | CLA  | ND   |
| 22  | B     | 1011 | CLA  | C8   |
| 22  | B     | 1011 | CLA  | CBD  |
| 22  | B     | 1011 | CLA  | ND   |
| 22  | B     | 1012 | CLA  | C8   |
| 22  | B     | 1012 | CLA  | ND   |
| 22  | B     | 1013 | CLA  | C8   |
| 22  | B     | 1013 | CLA  | ND   |
| 22  | B     | 1014 | CLA  | C8   |
| 22  | B     | 1014 | CLA  | ND   |
| 22  | B     | 1015 | CLA  | C8   |
| 22  | B     | 1015 | CLA  | ND   |
| 22  | B     | 1016 | CLA  | ND   |
| 22  | B     | 1018 | CLA  | C8   |
| 22  | B     | 1018 | CLA  | ND   |
| 22  | B     | 1019 | CLA  | C13  |
| 22  | B     | 1019 | CLA  | ND   |
| 22  | B     | 1020 | CLA  | C8   |
| 22  | B     | 1020 | CLA  | C13  |
| 22  | B     | 1020 | CLA  | ND   |
| 22  | B     | 1021 | CLA  | C8   |
| 22  | B     | 1021 | CLA  | ND   |
| 22  | B     | 1022 | CLA  | C13  |
| 22  | B     | 1022 | CLA  | CBD  |
| 22  | B     | 1022 | CLA  | ND   |
| 22  | B     | 1023 | CLA  | C8   |
| 22  | B     | 1023 | CLA  | C13  |
| 22  | B     | 1023 | CLA  | ND   |
| 22  | B     | 1024 | CLA  | ND   |
| 22  | C     | 1025 | CLA  | C8   |
| 22  | C     | 1025 | CLA  | ND   |
| 22  | C     | 1026 | CLA  | ND   |
| 22  | C     | 1027 | CLA  | C8   |
| 22  | C     | 1027 | CLA  | C13  |
| 22  | C     | 1027 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | C     | 1028 | CLA  | C8   |
| 22  | C     | 1028 | CLA  | ND   |
| 22  | C     | 1029 | CLA  | C8   |
| 22  | C     | 1029 | CLA  | C3A  |
| 22  | C     | 1029 | CLA  | ND   |
| 22  | C     | 1030 | CLA  | C8   |
| 22  | C     | 1030 | CLA  | ND   |
| 22  | C     | 1031 | CLA  | C8   |
| 22  | C     | 1031 | CLA  | ND   |
| 22  | C     | 1032 | CLA  | C8   |
| 22  | C     | 1032 | CLA  | C13  |
| 22  | C     | 1032 | CLA  | ND   |
| 22  | C     | 1033 | CLA  | C8   |
| 22  | C     | 1033 | CLA  | ND   |
| 22  | C     | 1035 | CLA  | C8   |
| 22  | C     | 1035 | CLA  | ND   |
| 22  | C     | 1036 | CLA  | C8   |
| 22  | C     | 1036 | CLA  | ND   |
| 22  | C     | 1037 | CLA  | C8   |
| 22  | C     | 1037 | CLA  | ND   |
| 22  | D     | 1005 | CLA  | C8   |
| 22  | D     | 1005 | CLA  | ND   |
| 22  | D     | 1004 | CLA  | C8   |
| 22  | D     | 1004 | CLA  | ND   |
| 22  | D     | 1008 | CLA  | C8   |
| 22  | D     | 1008 | CLA  | C3A  |
| 22  | D     | 1008 | CLA  | ND   |
| 22  | H     | 1017 | CLA  | C8   |
| 22  | H     | 1017 | CLA  | ND   |
| 22  | K     | 1034 | CLA  | C2A  |
| 22  | K     | 1034 | CLA  | C8   |
| 22  | K     | 1034 | CLA  | C3A  |
| 22  | K     | 1034 | CLA  | C13  |
| 22  | K     | 1034 | CLA  | ND   |
| 22  | a     | 6003 | CLA  | C8   |
| 22  | a     | 6003 | CLA  | ND   |
| 22  | a     | 6006 | CLA  | C8   |
| 22  | a     | 6006 | CLA  | ND   |
| 22  | a     | 6007 | CLA  | ND   |
| 22  | b     | 6009 | CLA  | CBD  |
| 22  | b     | 6009 | CLA  | ND   |
| 22  | b     | 6010 | CLA  | C8   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | b     | 6010 | CLA  | ND   |
| 22  | b     | 6011 | CLA  | C8   |
| 22  | b     | 6011 | CLA  | CBD  |
| 22  | b     | 6011 | CLA  | ND   |
| 22  | b     | 6012 | CLA  | C8   |
| 22  | b     | 6012 | CLA  | ND   |
| 22  | b     | 6013 | CLA  | C8   |
| 22  | b     | 6013 | CLA  | ND   |
| 22  | b     | 6014 | CLA  | C8   |
| 22  | b     | 6014 | CLA  | ND   |
| 22  | b     | 6015 | CLA  | C8   |
| 22  | b     | 6015 | CLA  | ND   |
| 22  | b     | 6016 | CLA  | ND   |
| 22  | b     | 6018 | CLA  | C8   |
| 22  | b     | 6018 | CLA  | ND   |
| 22  | b     | 6019 | CLA  | C13  |
| 22  | b     | 6019 | CLA  | ND   |
| 22  | b     | 6020 | CLA  | C8   |
| 22  | b     | 6020 | CLA  | C13  |
| 22  | b     | 6020 | CLA  | ND   |
| 22  | b     | 6021 | CLA  | C8   |
| 22  | b     | 6021 | CLA  | ND   |
| 22  | b     | 6022 | CLA  | C13  |
| 22  | b     | 6022 | CLA  | CBD  |
| 22  | b     | 6022 | CLA  | ND   |
| 22  | b     | 6023 | CLA  | C8   |
| 22  | b     | 6023 | CLA  | C13  |
| 22  | b     | 6023 | CLA  | ND   |
| 22  | b     | 6024 | CLA  | ND   |
| 22  | c     | 6025 | CLA  | C8   |
| 22  | c     | 6025 | CLA  | ND   |
| 22  | c     | 6026 | CLA  | ND   |
| 22  | c     | 6027 | CLA  | C8   |
| 22  | c     | 6027 | CLA  | C13  |
| 22  | c     | 6027 | CLA  | ND   |
| 22  | c     | 6028 | CLA  | C8   |
| 22  | c     | 6028 | CLA  | ND   |
| 22  | c     | 6029 | CLA  | C8   |
| 22  | c     | 6029 | CLA  | C3A  |
| 22  | c     | 6029 | CLA  | ND   |
| 22  | c     | 6030 | CLA  | C8   |
| 22  | c     | 6030 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | c     | 6031 | CLA  | C8   |
| 22  | c     | 6031 | CLA  | ND   |
| 22  | c     | 6032 | CLA  | C8   |
| 22  | c     | 6032 | CLA  | C13  |
| 22  | c     | 6032 | CLA  | ND   |
| 22  | c     | 6033 | CLA  | C8   |
| 22  | c     | 6033 | CLA  | ND   |
| 22  | c     | 6035 | CLA  | C8   |
| 22  | c     | 6035 | CLA  | ND   |
| 22  | c     | 6036 | CLA  | C8   |
| 22  | c     | 6036 | CLA  | ND   |
| 22  | c     | 6037 | CLA  | C8   |
| 22  | c     | 6037 | CLA  | ND   |
| 22  | d     | 6005 | CLA  | C8   |
| 22  | d     | 6005 | CLA  | ND   |
| 22  | d     | 6004 | CLA  | C8   |
| 22  | d     | 6004 | CLA  | ND   |
| 22  | d     | 6008 | CLA  | C8   |
| 22  | d     | 6008 | CLA  | C3A  |
| 22  | d     | 6008 | CLA  | ND   |
| 22  | h     | 6017 | CLA  | C8   |
| 22  | h     | 6017 | CLA  | ND   |
| 22  | k     | 6034 | CLA  | C2A  |
| 22  | k     | 6034 | CLA  | C8   |
| 22  | k     | 6034 | CLA  | C3A  |
| 22  | k     | 6034 | CLA  | C13  |
| 22  | k     | 6034 | CLA  | ND   |
| 23  | A     | 1038 | PHO  | C8   |
| 23  | D     | 1039 | PHO  | C8   |
| 23  | D     | 1039 | PHO  | C13  |
| 23  | D     | 1039 | PHO  | C3A  |
| 23  | a     | 6038 | PHO  | C8   |
| 23  | d     | 6039 | PHO  | C8   |
| 23  | d     | 6039 | PHO  | C13  |
| 23  | d     | 6039 | PHO  | C3A  |

All (2320) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1003 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1003 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1003 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1003 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1003 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1006 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1006 | CLA  | C4C-C3C-CAC-CBC |
| 22  | A     | 1007 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1007 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1007 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1007 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1007 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1007 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1009 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1009 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1009 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1009 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1011 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1011 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1012 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1012 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1012 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1013 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1013 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 1013 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 1013 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1013 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1014 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1014 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1014 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1014 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1014 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1015 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1015 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1015 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 1015 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 1015 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1016 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1016 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1016 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1016 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1018 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 1019 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1019 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1019 | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1019 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 1020 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1020 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1020 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1020 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1020 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 1020 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1021 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 1021 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 1021 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1022 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1023 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 1023 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 1024 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1024 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 1025 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 1025 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 1025 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 1025 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 1026 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 1026 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 1026 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 1026 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 1026 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 1027 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 1027 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1028 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 1028 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 1030 | CLA  | C2C-C3C-CAC-CBC |
| 22  | C     | 1030 | CLA  | C4C-C3C-CAC-CBC |
| 22  | C     | 1030 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 1030 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1030 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1031 | CLA  | C2C-C3C-CAC-CBC |
| 22  | C     | 1031 | CLA  | C4C-C3C-CAC-CBC |
| 22  | C     | 1031 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 1032 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 1032 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 1033 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 1033 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 1033 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 1035 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 1035 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 1036 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 1036 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 1036 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 1037 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 1037 | CLA  | C4C-C3C-CAC-CBC |
| 22  | D     | 1005 | CLA  | C1A-C2A-CAA-CBA |
| 22  | D     | 1005 | CLA  | C3A-C2A-CAA-CBA |
| 22  | D     | 1004 | CLA  | CAD-CBD-CGD-O2D |
| 22  | D     | 1008 | CLA  | CBD-CGD-O2D-CED |
| 22  | D     | 1008 | CLA  | C2-C3-C5-C6     |
| 22  | D     | 1008 | CLA  | C4-C3-C5-C6     |
| 22  | H     | 1017 | CLA  | CHA-CBD-CGD-O2D |
| 22  | K     | 1034 | CLA  | C4B-C3B-CAB-CBB |
| 22  | K     | 1034 | CLA  | CAD-CBD-CGD-O2D |
| 22  | K     | 1034 | CLA  | O2A-C1-C2-C3    |
| 22  | a     | 6003 | CLA  | C1A-C2A-CAA-CBA |
| 22  | a     | 6003 | CLA  | C2B-C3B-CAB-CBB |
| 22  | a     | 6003 | CLA  | C4B-C3B-CAB-CBB |
| 22  | a     | 6003 | CLA  | CBD-CGD-O2D-CED |
| 22  | a     | 6003 | CLA  | O1D-CGD-O2D-CED |
| 22  | a     | 6006 | CLA  | C1A-C2A-CAA-CBA |
| 22  | a     | 6006 | CLA  | C4C-C3C-CAC-CBC |
| 22  | a     | 6007 | CLA  | C1A-C2A-CAA-CBA |
| 22  | a     | 6007 | CLA  | C3A-C2A-CAA-CBA |
| 22  | a     | 6007 | CLA  | C2B-C3B-CAB-CBB |
| 22  | a     | 6007 | CLA  | C4B-C3B-CAB-CBB |
| 22  | a     | 6007 | CLA  | CBD-CGD-O2D-CED |
| 22  | a     | 6007 | CLA  | C11-C10-C8-C7   |
| 22  | a     | 6007 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6009 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6009 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6009 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6009 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6011 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6011 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6012 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6012 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6012 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6013 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6013 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 6013 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | b     | 6013 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6013 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6014 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6014 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6014 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6014 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6014 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6015 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6015 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6015 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 6015 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 6015 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6016 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6016 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6016 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6016 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 6018 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 6019 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6019 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6019 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 6019 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 6020 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6020 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6020 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6020 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6020 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 6020 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6021 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 6021 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 6021 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6022 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6023 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 6023 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 6024 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6024 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 6025 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 6025 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 6025 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 6025 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6026 | CLA  | C2-C1-O2A-CGA   |
| 22  | c     | 6026 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 6026 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | c     | 6026 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6026 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 6027 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6027 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 6028 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 6028 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 6030 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6030 | CLA  | C4C-C3C-CAC-CBC |
| 22  | c     | 6030 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6030 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 6030 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 6030 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 6031 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6031 | CLA  | C4C-C3C-CAC-CBC |
| 22  | c     | 6031 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 6032 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 6032 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 6033 | CLA  | C2-C1-O2A-CGA   |
| 22  | c     | 6033 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 6033 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6035 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 6035 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 6036 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 6036 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 6036 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6037 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 6037 | CLA  | C4C-C3C-CAC-CBC |
| 22  | d     | 6005 | CLA  | C1A-C2A-CAA-CBA |
| 22  | d     | 6005 | CLA  | C3A-C2A-CAA-CBA |
| 22  | d     | 6004 | CLA  | CAD-CBD-CGD-O2D |
| 22  | d     | 6008 | CLA  | CBD-CGD-O2D-CED |
| 22  | d     | 6008 | CLA  | C2-C3-C5-C6     |
| 22  | d     | 6008 | CLA  | C4-C3-C5-C6     |
| 22  | h     | 6017 | CLA  | CHA-CBD-CGD-O2D |
| 22  | k     | 6034 | CLA  | C4B-C3B-CAB-CBB |
| 22  | k     | 6034 | CLA  | CAD-CBD-CGD-O2D |
| 22  | k     | 6034 | CLA  | O2A-C1-C2-C3    |
| 23  | A     | 1038 | PHO  | C3A-C2A-CAA-CBA |
| 23  | A     | 1038 | PHO  | C2C-C3C-CAC-CBC |
| 23  | A     | 1038 | PHO  | CAD-CBD-CGD-O1D |
| 23  | A     | 1038 | PHO  | CAD-CBD-CGD-O2D |
| 23  | A     | 1038 | PHO  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | A     | 1038 | PHO  | C6-C7-C8-C9     |
| 23  | D     | 1039 | PHO  | C2C-C3C-CAC-CBC |
| 23  | D     | 1039 | PHO  | O2A-C1-C2-C3    |
| 23  | D     | 1039 | PHO  | C11-C10-C8-C9   |
| 23  | a     | 6038 | PHO  | C3A-C2A-CAA-CBA |
| 23  | a     | 6038 | PHO  | C2C-C3C-CAC-CBC |
| 23  | a     | 6038 | PHO  | CAD-CBD-CGD-O1D |
| 23  | a     | 6038 | PHO  | CAD-CBD-CGD-O2D |
| 23  | a     | 6038 | PHO  | CBD-CGD-O2D-CED |
| 23  | a     | 6038 | PHO  | C6-C7-C8-C9     |
| 23  | d     | 6039 | PHO  | C2C-C3C-CAC-CBC |
| 23  | d     | 6039 | PHO  | O2A-C1-C2-C3    |
| 23  | d     | 6039 | PHO  | C11-C10-C8-C9   |
| 24  | D     | 1042 | PQ9  | C30-C31-C32-C33 |
| 24  | D     | 1042 | PQ9  | C39-C38-C40-C41 |
| 24  | d     | 6042 | PQ9  | C30-C31-C32-C33 |
| 24  | d     | 6042 | PQ9  | C39-C38-C40-C41 |
| 25  | A     | 1044 | BCR  | C6-C7-C8-C9     |
| 25  | A     | 1044 | BCR  | C10-C11-C12-C13 |
| 25  | A     | 1044 | BCR  | C20-C21-C22-C23 |
| 25  | A     | 1044 | BCR  | C20-C21-C22-C37 |
| 25  | B     | 1045 | BCR  | C7-C8-C9-C34    |
| 25  | B     | 1045 | BCR  | C9-C10-C11-C12  |
| 25  | B     | 1045 | BCR  | C10-C11-C12-C13 |
| 25  | B     | 1045 | BCR  | C14-C15-C16-C17 |
| 25  | B     | 1045 | BCR  | C15-C16-C17-C18 |
| 25  | B     | 1045 | BCR  | C16-C17-C18-C19 |
| 25  | B     | 1045 | BCR  | C16-C17-C18-C36 |
| 25  | B     | 1045 | BCR  | C18-C19-C20-C21 |
| 25  | B     | 1045 | BCR  | C19-C20-C21-C22 |
| 25  | B     | 1045 | BCR  | C23-C24-C25-C26 |
| 25  | B     | 1045 | BCR  | C23-C24-C25-C30 |
| 25  | B     | 1047 | BCR  | C1-C6-C7-C8     |
| 25  | B     | 1047 | BCR  | C5-C6-C7-C8     |
| 25  | B     | 1047 | BCR  | C17-C18-C19-C20 |
| 25  | B     | 1047 | BCR  | C36-C18-C19-C20 |
| 25  | B     | 1047 | BCR  | C18-C19-C20-C21 |
| 25  | B     | 1047 | BCR  | C20-C21-C22-C23 |
| 25  | B     | 1047 | BCR  | C20-C21-C22-C37 |
| 25  | B     | 1048 | BCR  | C10-C11-C12-C13 |
| 25  | B     | 1048 | BCR  | C14-C15-C16-C17 |
| 25  | B     | 1048 | BCR  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 1048 | BCR  | C18-C19-C20-C21 |
| 25  | C     | 1052 | BCR  | C7-C8-C9-C10    |
| 25  | C     | 1052 | BCR  | C10-C11-C12-C13 |
| 25  | C     | 1052 | BCR  | C23-C24-C25-C26 |
| 25  | C     | 1052 | BCR  | C23-C24-C25-C30 |
| 25  | C     | 1054 | BCR  | C1-C6-C7-C8     |
| 25  | C     | 1054 | BCR  | C5-C6-C7-C8     |
| 25  | C     | 1054 | BCR  | C7-C8-C9-C34    |
| 25  | C     | 1054 | BCR  | C10-C11-C12-C13 |
| 25  | C     | 1054 | BCR  | C14-C15-C16-C17 |
| 25  | C     | 1054 | BCR  | C15-C16-C17-C18 |
| 25  | C     | 1054 | BCR  | C18-C19-C20-C21 |
| 25  | D     | 1050 | BCR  | C5-C6-C7-C8     |
| 25  | D     | 1050 | BCR  | C10-C11-C12-C13 |
| 25  | D     | 1050 | BCR  | C11-C12-C13-C14 |
| 25  | D     | 1050 | BCR  | C11-C12-C13-C35 |
| 25  | D     | 1050 | BCR  | C13-C14-C15-C16 |
| 25  | D     | 1050 | BCR  | C14-C15-C16-C17 |
| 25  | D     | 1050 | BCR  | C16-C17-C18-C19 |
| 25  | D     | 1050 | BCR  | C16-C17-C18-C36 |
| 25  | D     | 1050 | BCR  | C17-C18-C19-C20 |
| 25  | D     | 1050 | BCR  | C36-C18-C19-C20 |
| 25  | D     | 1050 | BCR  | C18-C19-C20-C21 |
| 25  | D     | 1050 | BCR  | C23-C24-C25-C26 |
| 25  | D     | 1050 | BCR  | C23-C24-C25-C30 |
| 25  | H     | 1049 | BCR  | C10-C11-C12-C13 |
| 25  | H     | 1049 | BCR  | C11-C12-C13-C14 |
| 25  | H     | 1049 | BCR  | C14-C15-C16-C17 |
| 25  | H     | 1049 | BCR  | C15-C16-C17-C18 |
| 25  | H     | 1049 | BCR  | C17-C18-C19-C20 |
| 25  | H     | 1049 | BCR  | C36-C18-C19-C20 |
| 25  | H     | 1049 | BCR  | C18-C19-C20-C21 |
| 25  | K     | 1051 | BCR  | C7-C8-C9-C10    |
| 25  | K     | 1051 | BCR  | C7-C8-C9-C34    |
| 25  | K     | 1051 | BCR  | C14-C15-C16-C17 |
| 25  | K     | 1051 | BCR  | C18-C19-C20-C21 |
| 25  | T     | 6046 | BCR  | C10-C11-C12-C13 |
| 25  | T     | 6046 | BCR  | C14-C15-C16-C17 |
| 25  | T     | 6046 | BCR  | C18-C19-C20-C21 |
| 25  | T     | 6046 | BCR  | C19-C20-C21-C22 |
| 25  | T     | 6048 | BCR  | C10-C11-C12-C13 |
| 25  | T     | 6048 | BCR  | C14-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | T     | 6048 | BCR  | C15-C16-C17-C18 |
| 25  | T     | 6048 | BCR  | C18-C19-C20-C21 |
| 25  | Z     | 1053 | BCR  | C6-C7-C8-C9     |
| 25  | Z     | 1053 | BCR  | C7-C8-C9-C10    |
| 25  | Z     | 1053 | BCR  | C10-C11-C12-C13 |
| 25  | Z     | 1053 | BCR  | C20-C21-C22-C37 |
| 25  | Z     | 1053 | BCR  | C23-C24-C25-C26 |
| 25  | Z     | 1053 | BCR  | C23-C24-C25-C30 |
| 25  | a     | 6044 | BCR  | C6-C7-C8-C9     |
| 25  | a     | 6044 | BCR  | C10-C11-C12-C13 |
| 25  | a     | 6044 | BCR  | C20-C21-C22-C23 |
| 25  | a     | 6044 | BCR  | C20-C21-C22-C37 |
| 25  | b     | 6045 | BCR  | C7-C8-C9-C34    |
| 25  | b     | 6045 | BCR  | C9-C10-C11-C12  |
| 25  | b     | 6045 | BCR  | C10-C11-C12-C13 |
| 25  | b     | 6045 | BCR  | C14-C15-C16-C17 |
| 25  | b     | 6045 | BCR  | C15-C16-C17-C18 |
| 25  | b     | 6045 | BCR  | C16-C17-C18-C19 |
| 25  | b     | 6045 | BCR  | C16-C17-C18-C36 |
| 25  | b     | 6045 | BCR  | C18-C19-C20-C21 |
| 25  | b     | 6045 | BCR  | C19-C20-C21-C22 |
| 25  | b     | 6045 | BCR  | C23-C24-C25-C26 |
| 25  | b     | 6045 | BCR  | C23-C24-C25-C30 |
| 25  | b     | 6047 | BCR  | C1-C6-C7-C8     |
| 25  | b     | 6047 | BCR  | C5-C6-C7-C8     |
| 25  | b     | 6047 | BCR  | C17-C18-C19-C20 |
| 25  | b     | 6047 | BCR  | C36-C18-C19-C20 |
| 25  | b     | 6047 | BCR  | C18-C19-C20-C21 |
| 25  | b     | 6047 | BCR  | C20-C21-C22-C23 |
| 25  | b     | 6047 | BCR  | C20-C21-C22-C37 |
| 25  | c     | 6054 | BCR  | C1-C6-C7-C8     |
| 25  | c     | 6054 | BCR  | C5-C6-C7-C8     |
| 25  | c     | 6054 | BCR  | C7-C8-C9-C34    |
| 25  | c     | 6054 | BCR  | C10-C11-C12-C13 |
| 25  | c     | 6054 | BCR  | C14-C15-C16-C17 |
| 25  | c     | 6054 | BCR  | C15-C16-C17-C18 |
| 25  | c     | 6054 | BCR  | C18-C19-C20-C21 |
| 25  | d     | 6050 | BCR  | C5-C6-C7-C8     |
| 25  | d     | 6050 | BCR  | C10-C11-C12-C13 |
| 25  | d     | 6050 | BCR  | C11-C12-C13-C14 |
| 25  | d     | 6050 | BCR  | C11-C12-C13-C35 |
| 25  | d     | 6050 | BCR  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | d     | 6050 | BCR  | C14-C15-C16-C17 |
| 25  | d     | 6050 | BCR  | C16-C17-C18-C19 |
| 25  | d     | 6050 | BCR  | C16-C17-C18-C36 |
| 25  | d     | 6050 | BCR  | C17-C18-C19-C20 |
| 25  | d     | 6050 | BCR  | C36-C18-C19-C20 |
| 25  | d     | 6050 | BCR  | C18-C19-C20-C21 |
| 25  | d     | 6050 | BCR  | C23-C24-C25-C26 |
| 25  | d     | 6050 | BCR  | C23-C24-C25-C30 |
| 25  | h     | 6049 | BCR  | C10-C11-C12-C13 |
| 25  | h     | 6049 | BCR  | C11-C12-C13-C14 |
| 25  | h     | 6049 | BCR  | C14-C15-C16-C17 |
| 25  | h     | 6049 | BCR  | C15-C16-C17-C18 |
| 25  | h     | 6049 | BCR  | C17-C18-C19-C20 |
| 25  | h     | 6049 | BCR  | C36-C18-C19-C20 |
| 25  | h     | 6049 | BCR  | C18-C19-C20-C21 |
| 25  | k     | 6052 | BCR  | C7-C8-C9-C10    |
| 25  | k     | 6052 | BCR  | C10-C11-C12-C13 |
| 25  | k     | 6052 | BCR  | C23-C24-C25-C26 |
| 25  | k     | 6052 | BCR  | C23-C24-C25-C30 |
| 25  | k     | 6051 | BCR  | C7-C8-C9-C10    |
| 25  | k     | 6051 | BCR  | C7-C8-C9-C34    |
| 25  | k     | 6051 | BCR  | C14-C15-C16-C17 |
| 25  | k     | 6051 | BCR  | C18-C19-C20-C21 |
| 25  | t     | 1046 | BCR  | C10-C11-C12-C13 |
| 25  | t     | 1046 | BCR  | C14-C15-C16-C17 |
| 25  | t     | 1046 | BCR  | C18-C19-C20-C21 |
| 25  | t     | 1046 | BCR  | C19-C20-C21-C22 |
| 25  | z     | 6053 | BCR  | C6-C7-C8-C9     |
| 25  | z     | 6053 | BCR  | C7-C8-C9-C10    |
| 25  | z     | 6053 | BCR  | C10-C11-C12-C13 |
| 25  | z     | 6053 | BCR  | C20-C21-C22-C37 |
| 25  | z     | 6053 | BCR  | C23-C24-C25-C26 |
| 25  | z     | 6053 | BCR  | C23-C24-C25-C30 |
| 26  | A     | 1063 | LHG  | O1-C1-C2-C3     |
| 26  | A     | 1063 | LHG  | O2-C2-C3-O3     |
| 26  | a     | 6063 | LHG  | O1-C1-C2-C3     |
| 26  | a     | 6063 | LHG  | O2-C2-C3-O3     |
| 28  | D     | 1059 | MGE  | C2B-C1B-O2G-C2G |
| 28  | D     | 1062 | MGE  | C2G-C3G-O3G-C1D |
| 28  | d     | 6059 | MGE  | C2B-C1B-O2G-C2G |
| 28  | d     | 6062 | MGE  | C2G-C3G-O3G-C1D |
| 29  | B     | 1058 | DGD  | O6D-C1D-O3G-C3G |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 29  | C     | 1055 | DGD  | C2B-C1B-O2G-C2G |
| 29  | C     | 1055 | DGD  | O6D-C1D-O3G-C3G |
| 29  | C     | 1056 | DGD  | C2B-C1B-O2G-C2G |
| 29  | C     | 1056 | DGD  | C1G-C2G-O2G-C1B |
| 29  | C     | 1057 | DGD  | O1G-C1G-C2G-O2G |
| 29  | b     | 6058 | DGD  | O6D-C1D-O3G-C3G |
| 29  | c     | 6055 | DGD  | C2B-C1B-O2G-C2G |
| 29  | c     | 6055 | DGD  | O6D-C1D-O3G-C3G |
| 29  | c     | 6056 | DGD  | C2B-C1B-O2G-C2G |
| 29  | c     | 6056 | DGD  | C1G-C2G-O2G-C1B |
| 29  | c     | 6057 | DGD  | O1G-C1G-C2G-O2G |
| 31  | F     | 1040 | HEM  | C2C-C3C-CAC-CBC |
| 31  | F     | 1040 | HEM  | C4C-C3C-CAC-CBC |
| 31  | f     | 6040 | HEM  | C2C-C3C-CAC-CBC |
| 31  | f     | 6040 | HEM  | C4C-C3C-CAC-CBC |
| 22  | B     | 1022 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1023 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6022 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6023 | CLA  | C4C-C3C-CAC-CBC |
| 22  | A     | 1006 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1014 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1022 | CLA  | C2C-C3C-CAC-CBC |
| 22  | C     | 1037 | CLA  | C2C-C3C-CAC-CBC |
| 22  | a     | 6006 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6014 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6022 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6037 | CLA  | C2C-C3C-CAC-CBC |
| 22  | A     | 1007 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1026 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1033 | CLA  | O1D-CGD-O2D-CED |
| 22  | D     | 1008 | CLA  | O1D-CGD-O2D-CED |
| 22  | a     | 6007 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 6026 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 6033 | CLA  | O1D-CGD-O2D-CED |
| 22  | d     | 6008 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1013 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1024 | CLA  | C4C-C3C-CAC-CBC |
| 22  | C     | 1027 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6013 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6024 | CLA  | C4C-C3C-CAC-CBC |
| 22  | c     | 6027 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1023 | CLA  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | K     | 1034 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6023 | CLA  | C2C-C3C-CAC-CBC |
| 22  | k     | 6034 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1012 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1014 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1015 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1019 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1024 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1025 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6012 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6014 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6015 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6019 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6024 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 6025 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1019 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1024 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 1029 | CLA  | CBD-CGD-O2D-CED |
| 22  | D     | 1005 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6019 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6024 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6029 | CLA  | CBD-CGD-O2D-CED |
| 22  | d     | 6005 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1010 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 1025 | CLA  | O1A-CGA-O2A-C1  |
| 22  | D     | 1008 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6010 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6025 | CLA  | O1A-CGA-O2A-C1  |
| 22  | d     | 6008 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 1036 | CLA  | C4C-C3C-CAC-CBC |
| 22  | c     | 6036 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1013 | CLA  | C2C-C3C-CAC-CBC |
| 22  | C     | 1027 | CLA  | C2C-C3C-CAC-CBC |
| 22  | C     | 1036 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6013 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6027 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6036 | CLA  | C2C-C3C-CAC-CBC |
| 23  | A     | 1038 | PHO  | O1D-CGD-O2D-CED |
| 23  | a     | 6038 | PHO  | O1D-CGD-O2D-CED |
| 22  | C     | 1030 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6030 | CLA  | C13-C15-C16-C17 |
| 23  | A     | 1038 | PHO  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | a     | 6038 | PHO  | C3-C5-C6-C7     |
| 22  | K     | 1034 | CLA  | C4C-C3C-CAC-CBC |
| 22  | k     | 6034 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1024 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6024 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1021 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1022 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6021 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6022 | CLA  | O1D-CGD-O2D-CED |
| 22  | d     | 6005 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1016 | CLA  | O1A-CGA-O2A-C1  |
| 22  | D     | 1004 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6016 | CLA  | O1A-CGA-O2A-C1  |
| 22  | d     | 6004 | CLA  | O1A-CGA-O2A-C1  |
| 28  | D     | 1062 | MGE  | O1A-C1A-O1G-C1G |
| 28  | d     | 6062 | MGE  | O1A-C1A-O1G-C1G |
| 22  | D     | 1008 | CLA  | C15-C16-C17-C18 |
| 22  | d     | 6008 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 1029 | CLA  | C4C-C3C-CAC-CBC |
| 22  | c     | 6029 | CLA  | C4C-C3C-CAC-CBC |
| 28  | B     | 1060 | MGE  | C4D-C5D-C6D-O5D |
| 28  | b     | 6060 | MGE  | C4D-C5D-C6D-O5D |
| 22  | C     | 1029 | CLA  | O1D-CGD-O2D-CED |
| 22  | D     | 1005 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 6029 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1029 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6029 | CLA  | C2C-C3C-CAC-CBC |
| 29  | B     | 1058 | DGD  | O6D-C5D-C6D-O5D |
| 29  | b     | 6058 | DGD  | O6D-C5D-C6D-O5D |
| 22  | D     | 1008 | CLA  | C4C-C3C-CAC-CBC |
| 22  | d     | 6008 | CLA  | C4C-C3C-CAC-CBC |
| 22  | D     | 1008 | CLA  | C2C-C3C-CAC-CBC |
| 22  | d     | 6008 | CLA  | C2C-C3C-CAC-CBC |
| 28  | D     | 1059 | MGE  | O1B-C1B-O2G-C2G |
| 28  | d     | 6059 | MGE  | O1B-C1B-O2G-C2G |
| 29  | C     | 1055 | DGD  | O1B-C1B-O2G-C2G |
| 29  | C     | 1056 | DGD  | O1B-C1B-O2G-C2G |
| 29  | c     | 6055 | DGD  | O1B-C1B-O2G-C2G |
| 29  | c     | 6056 | DGD  | O1B-C1B-O2G-C2G |
| 22  | B     | 1009 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1016 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 1027 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 1035 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 1036 | CLA  | C3-C5-C6-C7     |
| 22  | D     | 1008 | CLA  | C3-C5-C6-C7     |
| 22  | H     | 1017 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6009 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6016 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 6027 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 6035 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 6036 | CLA  | C3-C5-C6-C7     |
| 22  | d     | 6008 | CLA  | C3-C5-C6-C7     |
| 22  | h     | 6017 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1016 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 1029 | CLA  | CBA-CGA-O2A-C1  |
| 22  | D     | 1004 | CLA  | CBA-CGA-O2A-C1  |
| 22  | D     | 1008 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 6016 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 6029 | CLA  | CBA-CGA-O2A-C1  |
| 22  | d     | 6004 | CLA  | CBA-CGA-O2A-C1  |
| 22  | d     | 6008 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 1028 | CLA  | CBD-CGD-O2D-CED |
| 22  | K     | 1034 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6028 | CLA  | CBD-CGD-O2D-CED |
| 22  | k     | 6034 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1003 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1016 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1019 | CLA  | C2C-C3C-CAC-CBC |
| 22  | a     | 6003 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6016 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6019 | CLA  | C2C-C3C-CAC-CBC |
| 22  | A     | 1003 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1007 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1014 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1027 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1028 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1032 | CLA  | C4-C3-C5-C6     |
| 22  | D     | 1005 | CLA  | C4-C3-C5-C6     |
| 22  | H     | 1017 | CLA  | C4-C3-C5-C6     |
| 22  | K     | 1034 | CLA  | C4-C3-C5-C6     |
| 22  | a     | 6003 | CLA  | C4-C3-C5-C6     |
| 22  | a     | 6007 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 6014 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 6027 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | c     | 6028 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 6032 | CLA  | C4-C3-C5-C6     |
| 22  | d     | 6005 | CLA  | C4-C3-C5-C6     |
| 22  | h     | 6017 | CLA  | C4-C3-C5-C6     |
| 22  | k     | 6034 | CLA  | C4-C3-C5-C6     |
| 24  | A     | 1043 | PQ9  | C14-C13-C15-C16 |
| 24  | A     | 1043 | PQ9  | C29-C28-C30-C31 |
| 24  | D     | 1042 | PQ9  | C19-C18-C20-C21 |
| 24  | a     | 6043 | PQ9  | C14-C13-C15-C16 |
| 24  | a     | 6043 | PQ9  | C29-C28-C30-C31 |
| 24  | d     | 6042 | PQ9  | C19-C18-C20-C21 |
| 22  | A     | 1007 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 1027 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 1030 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 1032 | CLA  | C2-C3-C5-C6     |
| 22  | D     | 1005 | CLA  | C2-C3-C5-C6     |
| 22  | H     | 1017 | CLA  | C2-C3-C5-C6     |
| 22  | a     | 6007 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 6027 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 6032 | CLA  | C2-C3-C5-C6     |
| 22  | d     | 6005 | CLA  | C2-C3-C5-C6     |
| 22  | h     | 6017 | CLA  | C2-C3-C5-C6     |
| 24  | A     | 1043 | PQ9  | C12-C13-C15-C16 |
| 24  | D     | 1042 | PQ9  | C17-C18-C20-C21 |
| 24  | D     | 1042 | PQ9  | C37-C38-C40-C41 |
| 24  | a     | 6043 | PQ9  | C12-C13-C15-C16 |
| 24  | d     | 6042 | PQ9  | C17-C18-C20-C21 |
| 24  | d     | 6042 | PQ9  | C37-C38-C40-C41 |
| 22  | A     | 1003 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1012 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1019 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1021 | CLA  | C2A-CAA-CBA-CGA |
| 22  | a     | 6003 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6012 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6019 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6021 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1023 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1024 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 1028 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 1029 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6023 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6024 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | c     | 6028 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 6029 | CLA  | C3-C5-C6-C7     |
| 31  | F     | 1040 | HEM  | C3A-C2A-CAA-CBA |
| 31  | f     | 6040 | HEM  | C3A-C2A-CAA-CBA |
| 22  | A     | 1006 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1009 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 1025 | CLA  | CBA-CGA-O2A-C1  |
| 22  | a     | 6006 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 6009 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 6025 | CLA  | CBA-CGA-O2A-C1  |
| 28  | D     | 1062 | MGE  | C2A-C1A-O1G-C1G |
| 28  | d     | 6062 | MGE  | C2A-C1A-O1G-C1G |
| 25  | B     | 1047 | BCR  | C15-C16-C17-C18 |
| 25  | C     | 1052 | BCR  | C19-C20-C21-C22 |
| 25  | C     | 1054 | BCR  | C19-C20-C21-C22 |
| 25  | D     | 1050 | BCR  | C9-C10-C11-C12  |
| 25  | D     | 1050 | BCR  | C15-C16-C17-C18 |
| 25  | H     | 1049 | BCR  | C19-C20-C21-C22 |
| 25  | K     | 1051 | BCR  | C13-C14-C15-C16 |
| 25  | K     | 1051 | BCR  | C15-C16-C17-C18 |
| 25  | T     | 6046 | BCR  | C15-C16-C17-C18 |
| 25  | Z     | 1053 | BCR  | C19-C20-C21-C22 |
| 25  | b     | 6047 | BCR  | C15-C16-C17-C18 |
| 25  | c     | 6054 | BCR  | C19-C20-C21-C22 |
| 25  | d     | 6050 | BCR  | C9-C10-C11-C12  |
| 25  | d     | 6050 | BCR  | C15-C16-C17-C18 |
| 25  | h     | 6049 | BCR  | C19-C20-C21-C22 |
| 25  | k     | 6052 | BCR  | C19-C20-C21-C22 |
| 25  | k     | 6051 | BCR  | C13-C14-C15-C16 |
| 25  | k     | 6051 | BCR  | C15-C16-C17-C18 |
| 25  | t     | 1046 | BCR  | C15-C16-C17-C18 |
| 25  | z     | 6053 | BCR  | C19-C20-C21-C22 |
| 29  | C     | 1055 | DGD  | O1A-C1A-O1G-C1G |
| 29  | c     | 6055 | DGD  | O1A-C1A-O1G-C1G |
| 22  | B     | 1016 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6016 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1035 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6035 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1003 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1010 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 1028 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 6010 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | c     | 6028 | CLA  | CBA-CGA-O2A-C1  |
| 29  | C     | 1055 | DGD  | C2A-C1A-O1G-C1G |
| 29  | c     | 6055 | DGD  | C2A-C1A-O1G-C1G |
| 28  | B     | 1060 | MGE  | O6D-C5D-C6D-O5D |
| 28  | b     | 6060 | MGE  | O6D-C5D-C6D-O5D |
| 22  | C     | 1028 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6028 | CLA  | O1A-CGA-O2A-C1  |
| 22  | a     | 6003 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1013 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 6013 | CLA  | O1D-CGD-O2D-CED |
| 26  | A     | 1063 | LHG  | C8-C7-O7-C5     |
| 26  | a     | 6063 | LHG  | C8-C7-O7-C5     |
| 22  | B     | 1012 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6012 | CLA  | C2C-C3C-CAC-CBC |
| 29  | C     | 1055 | DGD  | O6D-C5D-C6D-O5D |
| 29  | C     | 1056 | DGD  | O6D-C5D-C6D-O5D |
| 29  | c     | 6055 | DGD  | O6D-C5D-C6D-O5D |
| 29  | c     | 6056 | DGD  | O6D-C5D-C6D-O5D |
| 22  | B     | 1019 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 1025 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6019 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 6025 | CLA  | C3-C5-C6-C7     |
| 29  | C     | 1056 | DGD  | C1A-C2A-C3A-C4A |
| 29  | c     | 6056 | DGD  | C1A-C2A-C3A-C4A |
| 29  | C     | 1056 | DGD  | C6B-C7B-C8B-C9B |
| 29  | c     | 6056 | DGD  | C6B-C7B-C8B-C9B |
| 22  | A     | 1006 | CLA  | CBD-CGD-O2D-CED |
| 22  | a     | 6006 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1016 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6016 | CLA  | C4C-C3C-CAC-CBC |
| 22  | A     | 1003 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1014 | CLA  | C2-C3-C5-C6     |
| 22  | K     | 1034 | CLA  | C2-C3-C5-C6     |
| 22  | a     | 6003 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 6014 | CLA  | C2-C3-C5-C6     |
| 22  | k     | 6034 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1009 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6009 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1009 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6009 | CLA  | O1A-CGA-O2A-C1  |
| 24  | A     | 1043 | PQ9  | C33-C35-C36-C37 |
| 24  | D     | 1042 | PQ9  | C28-C30-C31-C32 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | D     | 1042 | PQ9  | C33-C35-C36-C37 |
| 24  | a     | 6043 | PQ9  | C33-C35-C36-C37 |
| 24  | d     | 6042 | PQ9  | C28-C30-C31-C32 |
| 24  | d     | 6042 | PQ9  | C33-C35-C36-C37 |
| 31  | F     | 1040 | HEM  | C1A-C2A-CAA-CBA |
| 31  | f     | 6040 | HEM  | C1A-C2A-CAA-CBA |
| 28  | B     | 1060 | MGE  | C7A-C8A-C9A-CAA |
| 31  | F     | 1040 | HEM  | C3D-CAD-CBD-CGD |
| 31  | f     | 6040 | HEM  | C3D-CAD-CBD-CGD |
| 22  | A     | 1006 | CLA  | C2A-CAA-CBA-CGA |
| 22  | a     | 6006 | CLA  | C2A-CAA-CBA-CGA |
| 28  | b     | 6060 | MGE  | C7A-C8A-C9A-CAA |
| 29  | B     | 1058 | DGD  | O6E-C1E-O5D-C6D |
| 29  | b     | 6058 | DGD  | O6E-C1E-O5D-C6D |
| 28  | L     | 1061 | MGE  | C2A-C1A-O1G-C1G |
| 28  | l     | 6061 | MGE  | C2A-C1A-O1G-C1G |
| 29  | C     | 1056 | DGD  | CBB-CCB-CDB-CEB |
| 29  | c     | 6056 | DGD  | CBB-CCB-CDB-CEB |
| 29  | C     | 1056 | DGD  | O6E-C5E-C6E-O5E |
| 29  | c     | 6056 | DGD  | O6E-C5E-C6E-O5E |
| 22  | B     | 1019 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6019 | CLA  | C4C-C3C-CAC-CBC |
| 28  | B     | 1060 | MGE  | C4B-C5B-C6B-C7B |
| 28  | b     | 6060 | MGE  | C4B-C5B-C6B-C7B |
| 29  | C     | 1056 | DGD  | C7A-C8A-C9A-CAA |
| 22  | A     | 1006 | CLA  | O1A-CGA-O2A-C1  |
| 22  | a     | 6006 | CLA  | O1A-CGA-O2A-C1  |
| 26  | A     | 1063 | LHG  | C1-C2-C3-O3     |
| 26  | a     | 6063 | LHG  | C1-C2-C3-O3     |
| 22  | C     | 1027 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 6027 | CLA  | CBA-CGA-O2A-C1  |
| 29  | B     | 1058 | DGD  | C2A-C1A-O1G-C1G |
| 29  | b     | 6058 | DGD  | C2A-C1A-O1G-C1G |
| 29  | C     | 1055 | DGD  | C7A-C8A-C9A-CAA |
| 29  | c     | 6055 | DGD  | C7A-C8A-C9A-CAA |
| 29  | c     | 6056 | DGD  | C7A-C8A-C9A-CAA |
| 22  | B     | 1020 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 6020 | CLA  | CBD-CGD-O2D-CED |
| 28  | D     | 1059 | MGE  | C4D-C5D-C6D-O5D |
| 28  | d     | 6059 | MGE  | C4D-C5D-C6D-O5D |
| 26  | A     | 1063 | LHG  | C13-C14-C15-C16 |
| 26  | a     | 6063 | LHG  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | L     | 1061 | MGE  | C3B-C4B-C5B-C6B |
| 28  | l     | 6061 | MGE  | C3B-C4B-C5B-C6B |
| 29  | B     | 1058 | DGD  | C4D-C5D-C6D-O5D |
| 29  | C     | 1055 | DGD  | C4D-C5D-C6D-O5D |
| 29  | b     | 6058 | DGD  | C4D-C5D-C6D-O5D |
| 29  | c     | 6055 | DGD  | C4D-C5D-C6D-O5D |
| 26  | A     | 1063 | LHG  | C30-C31-C32-C33 |
| 26  | a     | 6063 | LHG  | C30-C31-C32-C33 |
| 22  | B     | 1015 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 6015 | CLA  | C4-C3-C5-C6     |
| 24  | A     | 1043 | PQ9  | C19-C18-C20-C21 |
| 24  | a     | 6043 | PQ9  | C19-C18-C20-C21 |
| 22  | B     | 1015 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 1028 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 6015 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 6028 | CLA  | C2-C3-C5-C6     |
| 24  | A     | 1043 | PQ9  | C27-C28-C30-C31 |
| 24  | a     | 6043 | PQ9  | C27-C28-C30-C31 |
| 22  | A     | 1006 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1006 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1009 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1011 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1011 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1012 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1013 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1018 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1019 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1021 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1022 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1022 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1022 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1023 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1025 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1025 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 1026 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1029 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 1030 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 1031 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1035 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 1036 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1037 | CLA  | C11-C12-C13-C14 |
| 22  | D     | 1005 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | H     | 1017 | CLA  | C6-C7-C8-C9     |
| 22  | K     | 1034 | CLA  | C6-C7-C8-C9     |
| 22  | K     | 1034 | CLA  | C14-C13-C15-C16 |
| 22  | a     | 6006 | CLA  | C6-C7-C8-C9     |
| 22  | a     | 6006 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6009 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6011 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 6011 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6012 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 6013 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6018 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6019 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6021 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6022 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 6022 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6022 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6023 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6025 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6025 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 6026 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6029 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 6030 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 6031 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6035 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 6036 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6037 | CLA  | C11-C12-C13-C14 |
| 22  | d     | 6005 | CLA  | C11-C12-C13-C14 |
| 22  | h     | 6017 | CLA  | C6-C7-C8-C9     |
| 22  | k     | 6034 | CLA  | C6-C7-C8-C9     |
| 22  | k     | 6034 | CLA  | C14-C13-C15-C16 |
| 23  | D     | 1039 | PHO  | C6-C7-C8-C9     |
| 23  | D     | 1039 | PHO  | C11-C12-C13-C14 |
| 23  | d     | 6039 | PHO  | C6-C7-C8-C9     |
| 23  | d     | 6039 | PHO  | C11-C12-C13-C14 |
| 22  | B     | 1009 | CLA  | C2C-C3C-CAC-CBC |
| 22  | b     | 6009 | CLA  | C2C-C3C-CAC-CBC |
| 22  | C     | 1029 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6029 | CLA  | O1A-CGA-O2A-C1  |
| 25  | A     | 1044 | BCR  | C11-C12-C13-C35 |
| 25  | B     | 1045 | BCR  | C37-C22-C23-C24 |
| 25  | B     | 1047 | BCR  | C7-C8-C9-C34    |
| 25  | B     | 1047 | BCR  | C11-C12-C13-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 1048 | BCR  | C7-C8-C9-C34    |
| 25  | C     | 1052 | BCR  | C7-C8-C9-C34    |
| 25  | H     | 1049 | BCR  | C7-C8-C9-C34    |
| 25  | H     | 1049 | BCR  | C11-C12-C13-C35 |
| 25  | K     | 1051 | BCR  | C11-C12-C13-C35 |
| 25  | T     | 6048 | BCR  | C7-C8-C9-C34    |
| 25  | Z     | 1053 | BCR  | C7-C8-C9-C34    |
| 25  | Z     | 1053 | BCR  | C37-C22-C23-C24 |
| 25  | a     | 6044 | BCR  | C11-C12-C13-C35 |
| 25  | b     | 6045 | BCR  | C37-C22-C23-C24 |
| 25  | b     | 6047 | BCR  | C7-C8-C9-C34    |
| 25  | b     | 6047 | BCR  | C11-C12-C13-C35 |
| 25  | h     | 6049 | BCR  | C7-C8-C9-C34    |
| 25  | h     | 6049 | BCR  | C11-C12-C13-C35 |
| 25  | k     | 6052 | BCR  | C7-C8-C9-C34    |
| 25  | k     | 6051 | BCR  | C11-C12-C13-C35 |
| 25  | z     | 6053 | BCR  | C7-C8-C9-C34    |
| 25  | z     | 6053 | BCR  | C37-C22-C23-C24 |
| 25  | A     | 1044 | BCR  | C11-C12-C13-C14 |
| 25  | B     | 1045 | BCR  | C7-C8-C9-C10    |
| 25  | B     | 1045 | BCR  | C21-C22-C23-C24 |
| 25  | B     | 1047 | BCR  | C7-C8-C9-C10    |
| 25  | B     | 1047 | BCR  | C11-C12-C13-C14 |
| 25  | B     | 1048 | BCR  | C7-C8-C9-C10    |
| 25  | C     | 1054 | BCR  | C7-C8-C9-C10    |
| 25  | K     | 1051 | BCR  | C11-C12-C13-C14 |
| 25  | T     | 6048 | BCR  | C7-C8-C9-C10    |
| 25  | Z     | 1053 | BCR  | C21-C22-C23-C24 |
| 25  | a     | 6044 | BCR  | C11-C12-C13-C14 |
| 25  | b     | 6045 | BCR  | C7-C8-C9-C10    |
| 25  | b     | 6045 | BCR  | C21-C22-C23-C24 |
| 25  | b     | 6047 | BCR  | C7-C8-C9-C10    |
| 25  | b     | 6047 | BCR  | C11-C12-C13-C14 |
| 25  | c     | 6054 | BCR  | C7-C8-C9-C10    |
| 25  | k     | 6051 | BCR  | C11-C12-C13-C14 |
| 25  | z     | 6053 | BCR  | C21-C22-C23-C24 |
| 22  | B     | 1018 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 1031 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6018 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 6031 | CLA  | C2A-CAA-CBA-CGA |
| 29  | B     | 1058 | DGD  | C6B-C7B-C8B-C9B |
| 29  | b     | 6058 | DGD  | C6B-C7B-C8B-C9B |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1015 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6015 | CLA  | O1A-CGA-O2A-C1  |
| 29  | B     | 1058 | DGD  | O1A-C1A-O1G-C1G |
| 29  | b     | 6058 | DGD  | O1A-C1A-O1G-C1G |
| 26  | A     | 1063 | LHG  | O9-C7-O7-C5     |
| 26  | a     | 6063 | LHG  | O9-C7-O7-C5     |
| 28  | D     | 1059 | MGE  | O6D-C5D-C6D-O5D |
| 28  | d     | 6059 | MGE  | O6D-C5D-C6D-O5D |
| 22  | B     | 1015 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 6015 | CLA  | CBA-CGA-O2A-C1  |
| 29  | C     | 1056 | DGD  | C8B-C9B-CAB-CBB |
| 29  | c     | 6056 | DGD  | C8B-C9B-CAB-CBB |
| 22  | B     | 1021 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6021 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6032 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1033 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 6033 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1003 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1010 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1018 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1037 | CLA  | C12-C13-C15-C16 |
| 22  | a     | 6003 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6010 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6018 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6037 | CLA  | C12-C13-C15-C16 |
| 29  | C     | 1056 | DGD  | CEB-CFB-CGB-CHB |
| 29  | c     | 6056 | DGD  | CEB-CFB-CGB-CHB |
| 25  | A     | 1044 | BCR  | C19-C20-C21-C22 |
| 25  | C     | 1052 | BCR  | C15-C16-C17-C18 |
| 25  | D     | 1050 | BCR  | C19-C20-C21-C22 |
| 25  | a     | 6044 | BCR  | C19-C20-C21-C22 |
| 25  | d     | 6050 | BCR  | C19-C20-C21-C22 |
| 25  | k     | 6052 | BCR  | C15-C16-C17-C18 |
| 24  | A     | 1043 | PQ9  | C13-C15-C16-C17 |
| 24  | A     | 1043 | PQ9  | C38-C40-C41-C42 |
| 24  | a     | 6043 | PQ9  | C13-C15-C16-C17 |
| 24  | a     | 6043 | PQ9  | C38-C40-C41-C42 |
| 22  | H     | 1017 | CLA  | C15-C16-C17-C18 |
| 22  | h     | 6017 | CLA  | C15-C16-C17-C18 |
| 29  | C     | 1056 | DGD  | C4E-C5E-C6E-O5E |
| 29  | c     | 6056 | DGD  | C4E-C5E-C6E-O5E |
| 22  | B     | 1011 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | H     | 1017 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6011 | CLA  | O1A-CGA-O2A-C1  |
| 31  | F     | 1040 | HEM  | C2A-CAA-CBA-CGA |
| 31  | f     | 6040 | HEM  | C2A-CAA-CBA-CGA |
| 22  | B     | 1013 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 1032 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 1036 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6013 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 6032 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 6036 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1007 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1026 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 1027 | CLA  | C10-C11-C12-C13 |
| 22  | a     | 6007 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6026 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6027 | CLA  | C10-C11-C12-C13 |
| 28  | D     | 1059 | MGE  | C1B-C2B-C3B-C4B |
| 28  | D     | 1062 | MGE  | C1A-C2A-C3A-C4A |
| 28  | d     | 6059 | MGE  | C1B-C2B-C3B-C4B |
| 28  | d     | 6062 | MGE  | C1A-C2A-C3A-C4A |
| 29  | B     | 1058 | DGD  | C1A-C2A-C3A-C4A |
| 29  | C     | 1057 | DGD  | C1A-C2A-C3A-C4A |
| 29  | b     | 6058 | DGD  | C1A-C2A-C3A-C4A |
| 29  | c     | 6057 | DGD  | C1A-C2A-C3A-C4A |
| 22  | h     | 6017 | CLA  | O1A-CGA-O2A-C1  |
| 22  | K     | 1034 | CLA  | C3-C5-C6-C7     |
| 22  | k     | 6034 | CLA  | C3-C5-C6-C7     |
| 28  | D     | 1062 | MGE  | O6D-C1D-O3G-C3G |
| 28  | d     | 6062 | MGE  | O6D-C1D-O3G-C3G |
| 29  | C     | 1057 | DGD  | O6D-C1D-O3G-C3G |
| 29  | c     | 6057 | DGD  | O6D-C1D-O3G-C3G |
| 28  | L     | 1061 | MGE  | CBB-CCB-CDB-CEB |
| 28  | l     | 6061 | MGE  | CBB-CCB-CDB-CEB |
| 22  | B     | 1013 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1015 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1020 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1021 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1024 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1030 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 1032 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6013 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6015 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | b     | 6020 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6021 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6024 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6030 | CLA  | C8-C10-C11-C12  |
| 23  | A     | 1038 | PHO  | C13-C15-C16-C17 |
| 23  | a     | 6038 | PHO  | C13-C15-C16-C17 |
| 22  | D     | 1005 | CLA  | C2C-C3C-CAC-CBC |
| 22  | d     | 6005 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6037 | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 1063 | LHG  | C35-C36-C37-C38 |
| 26  | a     | 6063 | LHG  | C35-C36-C37-C38 |
| 28  | L     | 1061 | MGE  | O1A-C1A-O1G-C1G |
| 28  | l     | 6061 | MGE  | O1A-C1A-O1G-C1G |
| 28  | L     | 1061 | MGE  | C1A-C2A-C3A-C4A |
| 28  | l     | 6061 | MGE  | C1A-C2A-C3A-C4A |
| 22  | B     | 1009 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 1032 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1033 | CLA  | C5-C6-C7-C8     |
| 22  | D     | 1004 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6009 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6033 | CLA  | C5-C6-C7-C8     |
| 22  | d     | 6004 | CLA  | C8-C10-C11-C12  |
| 28  | B     | 1060 | MGE  | CBB-CCB-CDB-CEB |
| 28  | b     | 6060 | MGE  | CBB-CCB-CDB-CEB |
| 22  | B     | 1014 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1020 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6014 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6020 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 1031 | CLA  | C13-C15-C16-C17 |
| 22  | H     | 1017 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 6031 | CLA  | C13-C15-C16-C17 |
| 22  | h     | 6017 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 1037 | CLA  | CBA-CGA-O2A-C1  |
| 22  | H     | 1017 | CLA  | CBA-CGA-O2A-C1  |
| 22  | h     | 6017 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1021 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 6021 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1013 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6013 | CLA  | C3-C5-C6-C7     |
| 29  | C     | 1057 | DGD  | O6D-C5D-C6D-O5D |
| 29  | c     | 6057 | DGD  | O6D-C5D-C6D-O5D |
| 25  | B     | 1047 | BCR  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 1048 | BCR  | C19-C20-C21-C22 |
| 25  | T     | 6048 | BCR  | C19-C20-C21-C22 |
| 25  | b     | 6047 | BCR  | C13-C14-C15-C16 |
| 22  | B     | 1023 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 6023 | CLA  | C10-C11-C12-C13 |
| 23  | A     | 1038 | PHO  | C2A-CAA-CBA-CGA |
| 23  | a     | 6038 | PHO  | C2A-CAA-CBA-CGA |
| 22  | C     | 1032 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 6032 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 1028 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 1029 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 1035 | CLA  | C13-C15-C16-C17 |
| 22  | D     | 1004 | CLA  | C13-C15-C16-C17 |
| 22  | D     | 1008 | CLA  | C10-C11-C12-C13 |
| 22  | H     | 1017 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6028 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 6029 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 6035 | CLA  | C13-C15-C16-C17 |
| 22  | d     | 6004 | CLA  | C13-C15-C16-C17 |
| 22  | d     | 6008 | CLA  | C10-C11-C12-C13 |
| 22  | h     | 6017 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1007 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1016 | CLA  | C5-C6-C7-C8     |
| 22  | a     | 6007 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6016 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1012 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6012 | CLA  | C4C-C3C-CAC-CBC |
| 29  | C     | 1057 | DGD  | C6B-C7B-C8B-C9B |
| 29  | c     | 6057 | DGD  | C6B-C7B-C8B-C9B |
| 22  | A     | 1006 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1010 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1026 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1027 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 1028 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 1030 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1037 | CLA  | C13-C15-C16-C17 |
| 22  | a     | 6006 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 6010 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6026 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6027 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 6028 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 6030 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | c     | 6037 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1007 | CLA  | CBA-CGA-O2A-C1  |
| 22  | a     | 6007 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1012 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 6012 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1029 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 6029 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1014 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6014 | CLA  | C3-C5-C6-C7     |
| 29  | B     | 1058 | DGD  | CFB-CGB-CHB-CIB |
| 29  | b     | 6058 | DGD  | CFB-CGB-CHB-CIB |
| 28  | D     | 1062 | MGE  | C2D-C1D-O3G-C3G |
| 28  | d     | 6062 | MGE  | C2D-C1D-O3G-C3G |
| 29  | B     | 1058 | DGD  | C2D-C1D-O3G-C3G |
| 29  | C     | 1057 | DGD  | C2D-C1D-O3G-C3G |
| 29  | C     | 1057 | DGD  | C2E-C1E-O5D-C6D |
| 29  | b     | 6058 | DGD  | C2D-C1D-O3G-C3G |
| 29  | c     | 6057 | DGD  | C2D-C1D-O3G-C3G |
| 29  | c     | 6057 | DGD  | C2E-C1E-O5D-C6D |
| 22  | C     | 1032 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1013 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1014 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6013 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6014 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1018 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 6018 | CLA  | C15-C16-C17-C18 |
| 25  | A     | 1044 | BCR  | C16-C17-C18-C36 |
| 25  | B     | 1047 | BCR  | C16-C17-C18-C36 |
| 25  | C     | 1052 | BCR  | C20-C21-C22-C37 |
| 25  | H     | 1049 | BCR  | C16-C17-C18-C36 |
| 25  | K     | 1051 | BCR  | C16-C17-C18-C36 |
| 25  | a     | 6044 | BCR  | C16-C17-C18-C36 |
| 25  | b     | 6047 | BCR  | C16-C17-C18-C36 |
| 25  | h     | 6049 | BCR  | C16-C17-C18-C36 |
| 25  | k     | 6052 | BCR  | C20-C21-C22-C37 |
| 25  | k     | 6051 | BCR  | C16-C17-C18-C36 |
| 22  | a     | 6006 | CLA  | C3-C5-C6-C7     |
| 28  | B     | 1060 | MGE  | C1B-C2B-C3B-C4B |
| 28  | b     | 6060 | MGE  | C1B-C2B-C3B-C4B |
| 22  | C     | 1037 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 6037 | CLA  | C8-C10-C11-C12  |
| 25  | A     | 1044 | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 1045 | BCR  | C36-C18-C19-C20 |
| 25  | D     | 1050 | BCR  | C7-C8-C9-C34    |
| 25  | a     | 6044 | BCR  | C7-C8-C9-C34    |
| 25  | b     | 6045 | BCR  | C36-C18-C19-C20 |
| 25  | d     | 6050 | BCR  | C7-C8-C9-C34    |
| 25  | A     | 1044 | BCR  | C7-C8-C9-C10    |
| 25  | H     | 1049 | BCR  | C7-C8-C9-C10    |
| 25  | a     | 6044 | BCR  | C7-C8-C9-C10    |
| 25  | h     | 6049 | BCR  | C7-C8-C9-C10    |
| 22  | C     | 1027 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6027 | CLA  | O1A-CGA-O2A-C1  |
| 22  | H     | 1017 | CLA  | C2A-CAA-CBA-CGA |
| 22  | h     | 6017 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 6032 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1020 | CLA  | O2A-C1-C2-C3    |
| 22  | B     | 1022 | CLA  | O2A-C1-C2-C3    |
| 22  | b     | 6020 | CLA  | O2A-C1-C2-C3    |
| 22  | b     | 6022 | CLA  | O2A-C1-C2-C3    |
| 26  | A     | 1063 | LHG  | C6-C5-O7-C7     |
| 26  | a     | 6063 | LHG  | C6-C5-O7-C7     |
| 28  | L     | 1061 | MGE  | C1G-C2G-O2G-C1B |
| 28  | l     | 6061 | MGE  | C1G-C2G-O2G-C1B |
| 22  | A     | 1007 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1016 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1018 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1028 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1031 | CLA  | C16-C17-C18-C20 |
| 22  | a     | 6007 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6016 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6018 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 6028 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 6031 | CLA  | C16-C17-C18-C20 |
| 28  | L     | 1061 | MGE  | C7A-C8A-C9A-CAA |
| 28  | l     | 6061 | MGE  | C7A-C8A-C9A-CAA |
| 22  | A     | 1006 | CLA  | C3-C5-C6-C7     |
| 25  | A     | 1044 | BCR  | C16-C17-C18-C19 |
| 25  | B     | 1047 | BCR  | C16-C17-C18-C19 |
| 25  | C     | 1052 | BCR  | C20-C21-C22-C23 |
| 25  | H     | 1049 | BCR  | C16-C17-C18-C19 |
| 25  | K     | 1051 | BCR  | C16-C17-C18-C19 |
| 25  | Z     | 1053 | BCR  | C20-C21-C22-C23 |
| 25  | a     | 6044 | BCR  | C16-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | b     | 6047 | BCR  | C16-C17-C18-C19 |
| 25  | h     | 6049 | BCR  | C16-C17-C18-C19 |
| 25  | k     | 6052 | BCR  | C20-C21-C22-C23 |
| 25  | k     | 6051 | BCR  | C16-C17-C18-C19 |
| 25  | z     | 6053 | BCR  | C20-C21-C22-C23 |
| 29  | C     | 1057 | DGD  | O6E-C1E-O5D-C6D |
| 29  | c     | 6057 | DGD  | O6E-C1E-O5D-C6D |
| 29  | B     | 1058 | DGD  | C2B-C1B-O2G-C2G |
| 29  | b     | 6058 | DGD  | C2B-C1B-O2G-C2G |
| 29  | C     | 1056 | DGD  | C4D-C5D-C6D-O5D |
| 29  | c     | 6056 | DGD  | C4D-C5D-C6D-O5D |
| 24  | A     | 1043 | PQ9  | C17-C18-C20-C21 |
| 24  | a     | 6043 | PQ9  | C17-C18-C20-C21 |
| 26  | A     | 1063 | LHG  | C24-C23-O8-C6   |
| 26  | a     | 6063 | LHG  | C24-C23-O8-C6   |
| 22  | B     | 1011 | CLA  | C10-C11-C12-C13 |
| 22  | H     | 1017 | CLA  | CBD-CGD-O2D-CED |
| 22  | h     | 6017 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 6032 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1021 | CLA  | C2-C1-O2A-CGA   |
| 22  | b     | 6021 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1011 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1021 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6011 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6021 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1033 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 6011 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6032 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 6033 | CLA  | C10-C11-C12-C13 |
| 29  | C     | 1057 | DGD  | C4D-C5D-C6D-O5D |
| 29  | c     | 6057 | DGD  | C4D-C5D-C6D-O5D |
| 22  | b     | 6011 | CLA  | O1D-CGD-O2D-CED |
| 25  | Z     | 1053 | BCR  | C14-C15-C16-C17 |
| 25  | z     | 6053 | BCR  | C14-C15-C16-C17 |
| 29  | C     | 1056 | DGD  | C5A-C6A-C7A-C8A |
| 29  | c     | 6056 | DGD  | C5A-C6A-C7A-C8A |
| 22  | B     | 1011 | CLA  | O1D-CGD-O2D-CED |
| 26  | A     | 1063 | LHG  | C7-C8-C9-C10    |
| 26  | a     | 6063 | LHG  | C7-C8-C9-C10    |
| 28  | D     | 1062 | MGE  | CAB-CBB-CCB-CDB |
| 28  | B     | 1060 | MGE  | C2A-C1A-O1G-C1G |
| 28  | b     | 6060 | MGE  | C2A-C1A-O1G-C1G |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | d     | 6062 | MGE  | CAB-CBB-CCB-CDB |
| 29  | B     | 1058 | DGD  | C2B-C3B-C4B-C5B |
| 29  | C     | 1057 | DGD  | C6A-C7A-C8A-C9A |
| 29  | b     | 6058 | DGD  | C6A-C7A-C8A-C9A |
| 29  | b     | 6058 | DGD  | C2B-C3B-C4B-C5B |
| 29  | c     | 6057 | DGD  | C6A-C7A-C8A-C9A |
| 26  | A     | 1063 | LHG  | O1-C1-C2-O2     |
| 26  | a     | 6063 | LHG  | O1-C1-C2-O2     |
| 29  | B     | 1058 | DGD  | C6A-C7A-C8A-C9A |
| 22  | C     | 1028 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 6028 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 1028 | CLA  | C4B-C3B-CAB-CBB |
| 22  | H     | 1017 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 6028 | CLA  | C4B-C3B-CAB-CBB |
| 22  | h     | 6017 | CLA  | C4B-C3B-CAB-CBB |
| 28  | D     | 1062 | MGE  | C1B-C2B-C3B-C4B |
| 28  | d     | 6062 | MGE  | C1B-C2B-C3B-C4B |
| 29  | C     | 1055 | DGD  | C5A-C6A-C7A-C8A |
| 29  | C     | 1057 | DGD  | C2A-C3A-C4A-C5A |
| 29  | c     | 6055 | DGD  | C5A-C6A-C7A-C8A |
| 29  | c     | 6057 | DGD  | C2A-C3A-C4A-C5A |
| 22  | B     | 1016 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1025 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1031 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1033 | CLA  | C16-C17-C18-C19 |
| 22  | D     | 1005 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6016 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 6025 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 6031 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 6033 | CLA  | C16-C17-C18-C19 |
| 22  | d     | 6005 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1019 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1024 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 1025 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6019 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6024 | CLA  | C15-C16-C17-C18 |
| 28  | L     | 1061 | MGE  | C2B-C1B-O2G-C2G |
| 28  | l     | 6061 | MGE  | C2B-C1B-O2G-C2G |
| 28  | L     | 1061 | MGE  | CCB-CDB-CEB-CFB |
| 28  | l     | 6061 | MGE  | CCB-CDB-CEB-CFB |
| 29  | C     | 1055 | DGD  | CBB-CCB-CDB-CEB |
| 29  | c     | 6055 | DGD  | CBB-CCB-CDB-CEB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1019 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 1028 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1028 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 1037 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 6019 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6028 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6028 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 6037 | CLA  | C11-C10-C8-C7   |
| 28  | B     | 1060 | MGE  | C8A-C9A-CAA-CBA |
| 28  | b     | 6060 | MGE  | C8A-C9A-CAA-CBA |
| 29  | C     | 1055 | DGD  | C2A-C3A-C4A-C5A |
| 29  | c     | 6055 | DGD  | C2A-C3A-C4A-C5A |
| 29  | C     | 1057 | DGD  | C2A-C1A-O1G-C1G |
| 29  | c     | 6057 | DGD  | C2A-C1A-O1G-C1G |
| 22  | B     | 1020 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 6020 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6025 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1006 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1007 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1014 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1021 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 1036 | CLA  | C3A-C2A-CAA-CBA |
| 22  | a     | 6006 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6014 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6021 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 6036 | CLA  | C3A-C2A-CAA-CBA |
| 28  | d     | 6062 | MGE  | C2B-C3B-C4B-C5B |
| 28  | D     | 1062 | MGE  | C2B-C3B-C4B-C5B |
| 22  | A     | 1007 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1018 | CLA  | C10-C11-C12-C13 |
| 22  | a     | 6007 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6018 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6032 | CLA  | C13-C15-C16-C17 |
| 28  | B     | 1060 | MGE  | C6A-C7A-C8A-C9A |
| 22  | B     | 1018 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 1032 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6018 | CLA  | C3-C5-C6-C7     |
| 28  | L     | 1061 | MGE  | C1B-C2B-C3B-C4B |
| 28  | l     | 6061 | MGE  | C1B-C2B-C3B-C4B |
| 22  | B     | 1019 | CLA  | C10-C11-C12-C13 |
| 28  | D     | 1059 | MGE  | C6A-C7A-C8A-C9A |
| 28  | d     | 6059 | MGE  | C6A-C7A-C8A-C9A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | b     | 6060 | MGE  | C6A-C7A-C8A-C9A |
| 29  | C     | 1055 | DGD  | C8A-C9A-CAA-CBA |
| 29  | c     | 6055 | DGD  | C8A-C9A-CAA-CBA |
| 29  | C     | 1056 | DGD  | C6A-C7A-C8A-C9A |
| 22  | C     | 1036 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 6019 | CLA  | C10-C11-C12-C13 |
| 29  | c     | 6056 | DGD  | C6A-C7A-C8A-C9A |
| 22  | D     | 1008 | CLA  | C16-C17-C18-C19 |
| 22  | d     | 6008 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1013 | CLA  | C2B-C3B-CAB-CBB |
| 22  | H     | 1017 | CLA  | C2B-C3B-CAB-CBB |
| 22  | K     | 1034 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6013 | CLA  | C2B-C3B-CAB-CBB |
| 22  | h     | 6017 | CLA  | C2B-C3B-CAB-CBB |
| 22  | k     | 6034 | CLA  | C2B-C3B-CAB-CBB |
| 25  | C     | 1052 | BCR  | C5-C6-C7-C8     |
| 25  | D     | 1050 | BCR  | C1-C6-C7-C8     |
| 25  | Z     | 1053 | BCR  | C1-C6-C7-C8     |
| 25  | Z     | 1053 | BCR  | C5-C6-C7-C8     |
| 25  | d     | 6050 | BCR  | C1-C6-C7-C8     |
| 25  | k     | 6052 | BCR  | C5-C6-C7-C8     |
| 25  | z     | 6053 | BCR  | C1-C6-C7-C8     |
| 25  | z     | 6053 | BCR  | C5-C6-C7-C8     |
| 29  | c     | 6057 | DGD  | C7B-C8B-C9B-CAB |
| 22  | C     | 1032 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1024 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6024 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 6036 | CLA  | C10-C11-C12-C13 |
| 26  | A     | 1063 | LHG  | C31-C32-C33-C34 |
| 26  | a     | 6063 | LHG  | C31-C32-C33-C34 |
| 29  | C     | 1057 | DGD  | CAA-CBA-CCA-CDA |
| 29  | C     | 1057 | DGD  | C7B-C8B-C9B-CAB |
| 29  | c     | 6057 | DGD  | C9A-CAA-CBA-CCA |
| 29  | c     | 6057 | DGD  | CAA-CBA-CCA-CDA |
| 22  | c     | 6032 | CLA  | C2C-C3C-CAC-CBC |
| 29  | C     | 1057 | DGD  | C9A-CAA-CBA-CCA |
| 22  | k     | 6034 | CLA  | C15-C16-C17-C18 |
| 26  | A     | 1063 | LHG  | O10-C23-O8-C6   |
| 26  | a     | 6063 | LHG  | O10-C23-O8-C6   |
| 28  | B     | 1060 | MGE  | O1A-C1A-O1G-C1G |
| 28  | b     | 6060 | MGE  | O1A-C1A-O1G-C1G |
| 28  | d     | 6059 | MGE  | C2A-C3A-C4A-C5A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 29  | B     | 1058 | DGD  | O1B-C1B-O2G-C2G |
| 29  | b     | 6058 | DGD  | O1B-C1B-O2G-C2G |
| 28  | B     | 1060 | MGE  | C4A-C5A-C6A-C7A |
| 28  | D     | 1059 | MGE  | C2A-C3A-C4A-C5A |
| 28  | b     | 6060 | MGE  | C4A-C5A-C6A-C7A |
| 29  | C     | 1055 | DGD  | C3B-C4B-C5B-C6B |
| 29  | c     | 6055 | DGD  | C3B-C4B-C5B-C6B |
| 25  | C     | 1052 | BCR  | C18-C19-C20-C21 |
| 25  | k     | 6052 | BCR  | C18-C19-C20-C21 |
| 22  | K     | 1034 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1012 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 6012 | CLA  | C2-C3-C5-C6     |
| 28  | D     | 1062 | MGE  | C6B-C7B-C8B-C9B |
| 28  | d     | 6062 | MGE  | C6B-C7B-C8B-C9B |
| 22  | K     | 1034 | CLA  | C11-C12-C13-C14 |
| 22  | k     | 6034 | CLA  | C11-C12-C13-C14 |
| 25  | C     | 1054 | BCR  | C6-C7-C8-C9     |
| 25  | K     | 1051 | BCR  | C6-C7-C8-C9     |
| 25  | c     | 6054 | BCR  | C6-C7-C8-C9     |
| 25  | k     | 6051 | BCR  | C6-C7-C8-C9     |
| 29  | C     | 1057 | DGD  | O1A-C1A-O1G-C1G |
| 29  | c     | 6057 | DGD  | O1A-C1A-O1G-C1G |
| 29  | C     | 1055 | DGD  | C4A-C5A-C6A-C7A |
| 29  | C     | 1056 | DGD  | C9B-CAB-CBB-CCB |
| 29  | c     | 6055 | DGD  | C4A-C5A-C6A-C7A |
| 29  | c     | 6056 | DGD  | C9B-CAB-CBB-CCB |
| 25  | K     | 1051 | BCR  | C9-C10-C11-C12  |
| 25  | k     | 6051 | BCR  | C9-C10-C11-C12  |
| 28  | B     | 1060 | MGE  | C2B-C1B-O2G-C2G |
| 28  | b     | 6060 | MGE  | C2B-C1B-O2G-C2G |
| 29  | C     | 1057 | DGD  | CFB-CGB-CHB-CIB |
| 29  | c     | 6057 | DGD  | CFB-CGB-CHB-CIB |
| 29  | C     | 1055 | DGD  | CAA-CBA-CCA-CDA |
| 29  | c     | 6055 | DGD  | CAA-CBA-CCA-CDA |
| 22  | B     | 1011 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1013 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 6013 | CLA  | C15-C16-C17-C18 |
| 28  | L     | 1061 | MGE  | O1B-C1B-O2G-C2G |
| 28  | l     | 6061 | MGE  | O1B-C1B-O2G-C2G |
| 22  | k     | 6034 | CLA  | O1D-CGD-O2D-CED |
| 29  | C     | 1056 | DGD  | CFB-CGB-CHB-CIB |
| 29  | c     | 6056 | DGD  | CFB-CGB-CHB-CIB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 1027 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 6011 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 6027 | CLA  | C15-C16-C17-C18 |
| 25  | C     | 1054 | BCR  | C36-C18-C19-C20 |
| 25  | c     | 6054 | BCR  | C36-C18-C19-C20 |
| 28  | D     | 1062 | MGE  | CBB-CCB-CDB-CEB |
| 28  | d     | 6062 | MGE  | CBB-CCB-CDB-CEB |
| 29  | C     | 1055 | DGD  | C9A-CAA-CBA-CCA |
| 25  | C     | 1054 | BCR  | C17-C18-C19-C20 |
| 25  | c     | 6054 | BCR  | C17-C18-C19-C20 |
| 29  | C     | 1055 | DGD  | CFB-CGB-CHB-CIB |
| 29  | c     | 6055 | DGD  | CFB-CGB-CHB-CIB |
| 29  | c     | 6055 | DGD  | C9A-CAA-CBA-CCA |
| 22  | B     | 1015 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 1026 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6015 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 6026 | CLA  | C2A-CAA-CBA-CGA |
| 22  | D     | 1008 | CLA  | C16-C17-C18-C20 |
| 22  | d     | 6008 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6010 | CLA  | O1D-CGD-O2D-CED |
| 29  | C     | 1056 | DGD  | CBA-CCA-CDA-CEA |
| 22  | K     | 1034 | CLA  | O1D-CGD-O2D-CED |
| 29  | C     | 1055 | DGD  | C7B-C8B-C9B-CAB |
| 29  | c     | 6055 | DGD  | C7B-C8B-C9B-CAB |
| 29  | c     | 6056 | DGD  | CBA-CCA-CDA-CEA |
| 29  | c     | 6057 | DGD  | C8A-C9A-CAA-CBA |
| 22  | B     | 1010 | CLA  | O1D-CGD-O2D-CED |
| 29  | C     | 1057 | DGD  | C8A-C9A-CAA-CBA |
| 22  | B     | 1016 | CLA  | C15-C16-C17-C18 |
| 28  | D     | 1062 | MGE  | C5B-C6B-C7B-C8B |
| 28  | d     | 6062 | MGE  | C7A-C8A-C9A-CAA |
| 28  | d     | 6062 | MGE  | C5B-C6B-C7B-C8B |
| 28  | D     | 1062 | MGE  | C7A-C8A-C9A-CAA |
| 22  | b     | 6024 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1007 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1012 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1013 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1018 | CLA  | C16-C17-C18-C20 |
| 22  | a     | 6007 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6012 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6013 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6018 | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 29  | C     | 1055 | DGD  | C1A-C2A-C3A-C4A |
| 29  | c     | 6055 | DGD  | C1A-C2A-C3A-C4A |
| 22  | B     | 1015 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1024 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6015 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6016 | CLA  | C15-C16-C17-C18 |
| 29  | C     | 1057 | DGD  | O2G-C2G-C3G-O3G |
| 29  | c     | 6057 | DGD  | O2G-C2G-C3G-O3G |
| 22  | B     | 1009 | CLA  | C4C-C3C-CAC-CBC |
| 22  | b     | 6009 | CLA  | C4C-C3C-CAC-CBC |
| 28  | D     | 1062 | MGE  | C9B-CAB-CBB-CCB |
| 28  | d     | 6062 | MGE  | C9B-CAB-CBB-CCB |
| 28  | D     | 1062 | MGE  | C4B-C5B-C6B-C7B |
| 28  | D     | 1062 | MGE  | C7B-C8B-C9B-CAB |
| 28  | d     | 6062 | MGE  | C4B-C5B-C6B-C7B |
| 28  | d     | 6062 | MGE  | C7B-C8B-C9B-CAB |
| 29  | C     | 1056 | DGD  | C8A-C9A-CAA-CBA |
| 29  | c     | 6056 | DGD  | C8A-C9A-CAA-CBA |
| 26  | A     | 1063 | LHG  | C15-C16-C17-C18 |
| 26  | a     | 6063 | LHG  | C15-C16-C17-C18 |
| 29  | B     | 1058 | DGD  | CAA-CBA-CCA-CDA |
| 29  | b     | 6058 | DGD  | CAA-CBA-CCA-CDA |
| 28  | D     | 1062 | MGE  | C3A-C4A-C5A-C6A |
| 28  | D     | 1062 | MGE  | C4A-C5A-C6A-C7A |
| 28  | d     | 6062 | MGE  | C4A-C5A-C6A-C7A |
| 22  | B     | 1011 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 1033 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 6011 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 6033 | CLA  | CBA-CGA-O2A-C1  |
| 28  | d     | 6062 | MGE  | C3A-C4A-C5A-C6A |
| 22  | C     | 1036 | CLA  | C15-C16-C17-C18 |
| 22  | H     | 1017 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 6036 | CLA  | C15-C16-C17-C18 |
| 22  | h     | 6017 | CLA  | C8-C10-C11-C12  |
| 29  | C     | 1057 | DGD  | CBB-CCB-CDB-CEB |
| 29  | c     | 6057 | DGD  | CBB-CCB-CDB-CEB |
| 22  | B     | 1011 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1013 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1021 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 1025 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 1028 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 1037 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | b     | 6011 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6013 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6021 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 6025 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 6028 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 6037 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 1032 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1020 | CLA  | C2C-C3C-CAC-CBC |
| 28  | B     | 1060 | MGE  | O1B-C1B-O2G-C2G |
| 28  | b     | 6060 | MGE  | O1B-C1B-O2G-C2G |
| 22  | A     | 1003 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1011 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1014 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1022 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 1027 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 1028 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 1035 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1037 | CLA  | C11-C12-C13-C15 |
| 22  | D     | 1005 | CLA  | C6-C7-C8-C10    |
| 22  | D     | 1008 | CLA  | C11-C10-C8-C7   |
| 22  | H     | 1017 | CLA  | C11-C12-C13-C15 |
| 22  | a     | 6003 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 6011 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6014 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 6022 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 6027 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6028 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6035 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6037 | CLA  | C11-C12-C13-C15 |
| 22  | d     | 6005 | CLA  | C6-C7-C8-C10    |
| 22  | d     | 6008 | CLA  | C11-C10-C8-C7   |
| 22  | h     | 6017 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6020 | CLA  | C2C-C3C-CAC-CBC |
| 28  | L     | 1061 | MGE  | C6B-C7B-C8B-C9B |
| 28  | l     | 6061 | MGE  | C6B-C7B-C8B-C9B |
| 29  | C     | 1056 | DGD  | C2A-C3A-C4A-C5A |
| 22  | A     | 1006 | CLA  | C4-C3-C5-C6     |
| 22  | a     | 6006 | CLA  | C4-C3-C5-C6     |
| 24  | D     | 1042 | PQ9  | C34-C33-C35-C36 |
| 24  | d     | 6042 | PQ9  | C34-C33-C35-C36 |
| 29  | c     | 6056 | DGD  | C2A-C3A-C4A-C5A |
| 22  | B     | 1018 | CLA  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | b     | 6018 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1010 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6010 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1003 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1003 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1016 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1018 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1021 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1023 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 1035 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 1037 | CLA  | C14-C13-C15-C16 |
| 22  | a     | 6003 | CLA  | C6-C7-C8-C9     |
| 22  | a     | 6003 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6016 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6018 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6021 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6023 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 6035 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 6037 | CLA  | C14-C13-C15-C16 |
| 29  | C     | 1056 | DGD  | C2E-C1E-O5D-C6D |
| 29  | c     | 6056 | DGD  | C2E-C1E-O5D-C6D |
| 28  | B     | 1060 | MGE  | C1G-C2G-C3G-O3G |
| 28  | D     | 1059 | MGE  | C1G-C2G-C3G-O3G |
| 28  | L     | 1061 | MGE  | O1G-C1G-C2G-C3G |
| 28  | b     | 6060 | MGE  | C1G-C2G-C3G-O3G |
| 28  | d     | 6059 | MGE  | C1G-C2G-C3G-O3G |
| 28  | l     | 6061 | MGE  | O1G-C1G-C2G-C3G |
| 29  | B     | 1058 | DGD  | O1G-C1G-C2G-C3G |
| 29  | C     | 1055 | DGD  | C1G-C2G-C3G-O3G |
| 29  | C     | 1056 | DGD  | O1G-C1G-C2G-C3G |
| 29  | C     | 1057 | DGD  | O1G-C1G-C2G-C3G |
| 29  | b     | 6058 | DGD  | O1G-C1G-C2G-C3G |
| 29  | c     | 6055 | DGD  | C1G-C2G-C3G-O3G |
| 29  | c     | 6056 | DGD  | O1G-C1G-C2G-C3G |
| 29  | c     | 6057 | DGD  | O1G-C1G-C2G-C3G |
| 22  | B     | 1015 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 6015 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1021 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 1033 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6021 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 6033 | CLA  | C16-C17-C18-C20 |
| 28  | L     | 1061 | MGE  | C9B-CAB-CBB-CCB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | l     | 6061 | MGE  | C9B-CAB-CBB-CCB |
| 22  | C     | 1037 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6037 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1006 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 1033 | CLA  | C2-C3-C5-C6     |
| 22  | a     | 6006 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 6033 | CLA  | C2-C3-C5-C6     |
| 24  | D     | 1042 | PQ9  | C32-C33-C35-C36 |
| 24  | d     | 6042 | PQ9  | C32-C33-C35-C36 |
| 22  | A     | 1007 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 1032 | CLA  | O1A-CGA-O2A-C1  |
| 22  | a     | 6007 | CLA  | O1A-CGA-O2A-C1  |
| 28  | d     | 6062 | MGE  | C3B-C4B-C5B-C6B |
| 26  | A     | 1063 | LHG  | C26-C27-C28-C29 |
| 26  | a     | 6063 | LHG  | C26-C27-C28-C29 |
| 28  | D     | 1062 | MGE  | C3B-C4B-C5B-C6B |
| 22  | c     | 6032 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1011 | CLA  | O2A-C1-C2-C3    |
| 22  | B     | 1013 | CLA  | O2A-C1-C2-C3    |
| 22  | C     | 1026 | CLA  | O2A-C1-C2-C3    |
| 22  | C     | 1036 | CLA  | O2A-C1-C2-C3    |
| 22  | b     | 6011 | CLA  | O2A-C1-C2-C3    |
| 22  | b     | 6013 | CLA  | O2A-C1-C2-C3    |
| 22  | c     | 6026 | CLA  | O2A-C1-C2-C3    |
| 22  | c     | 6036 | CLA  | O2A-C1-C2-C3    |
| 28  | B     | 1060 | MGE  | C3G-C2G-O2G-C1B |
| 28  | b     | 6060 | MGE  | C3G-C2G-O2G-C1B |
| 28  | B     | 1060 | MGE  | C3A-C4A-C5A-C6A |
| 28  | b     | 6060 | MGE  | C3A-C4A-C5A-C6A |
| 25  | K     | 1051 | BCR  | C19-C20-C21-C22 |
| 25  | k     | 6051 | BCR  | C19-C20-C21-C22 |
| 26  | A     | 1063 | LHG  | C9-C10-C11-C12  |
| 26  | A     | 1063 | LHG  | C10-C11-C12-C13 |
| 26  | a     | 6063 | LHG  | C10-C11-C12-C13 |
| 22  | B     | 1022 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 1036 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 6022 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 6036 | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 1063 | LHG  | C17-C18-C19-C20 |
| 26  | a     | 6063 | LHG  | C9-C10-C11-C12  |
| 26  | a     | 6063 | LHG  | C17-C18-C19-C20 |
| 29  | c     | 6055 | DGD  | C6B-C7B-C8B-C9B |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | D     | 1059 | MGE  | C6B-C7B-C8B-C9B |
| 28  | d     | 6059 | MGE  | C6B-C7B-C8B-C9B |
| 29  | C     | 1055 | DGD  | C6B-C7B-C8B-C9B |
| 28  | B     | 1060 | MGE  | C2B-C3B-C4B-C5B |
| 28  | b     | 6060 | MGE  | C2B-C3B-C4B-C5B |
| 29  | c     | 6055 | DGD  | CBA-CCA-CDA-CEA |
| 29  | C     | 1055 | DGD  | CBA-CCA-CDA-CEA |
| 29  | C     | 1056 | DGD  | C9A-CAA-CBA-CCA |
| 29  | C     | 1057 | DGD  | C3A-C4A-C5A-C6A |
| 29  | c     | 6056 | DGD  | C9A-CAA-CBA-CCA |
| 29  | c     | 6057 | DGD  | C3A-C4A-C5A-C6A |
| 29  | B     | 1058 | DGD  | O1G-C1G-C2G-O2G |
| 29  | b     | 6058 | DGD  | O1G-C1G-C2G-O2G |
| 28  | l     | 6061 | MGE  | C2A-C3A-C4A-C5A |
| 22  | D     | 1005 | CLA  | C4C-C3C-CAC-CBC |
| 28  | L     | 1061 | MGE  | C2A-C3A-C4A-C5A |
| 29  | C     | 1057 | DGD  | C4A-C5A-C6A-C7A |
| 29  | c     | 6057 | DGD  | C4A-C5A-C6A-C7A |
| 22  | d     | 6005 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1023 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6023 | CLA  | C8-C10-C11-C12  |
| 25  | A     | 1044 | BCR  | C15-C16-C17-C18 |
| 25  | B     | 1047 | BCR  | C9-C10-C11-C12  |
| 25  | a     | 6044 | BCR  | C15-C16-C17-C18 |
| 25  | b     | 6047 | BCR  | C9-C10-C11-C12  |
| 22  | B     | 1018 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1033 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 6018 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 6033 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1030 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 6030 | CLA  | C5-C6-C7-C8     |
| 28  | L     | 1061 | MGE  | C4D-C5D-C6D-O5D |
| 28  | l     | 6061 | MGE  | C4D-C5D-C6D-O5D |
| 28  | D     | 1059 | MGE  | C7A-C8A-C9A-CAA |
| 28  | d     | 6059 | MGE  | C7A-C8A-C9A-CAA |
| 22  | A     | 1003 | CLA  | C3-C5-C6-C7     |
| 22  | a     | 6003 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1009 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1010 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1011 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1012 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1014 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1018 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1023 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 1028 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 1030 | CLA  | C6-C7-C8-C9     |
| 22  | D     | 1005 | CLA  | C6-C7-C8-C9     |
| 22  | H     | 1017 | CLA  | C11-C12-C13-C14 |
| 22  | H     | 1017 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6009 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6010 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 6011 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6012 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6014 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6018 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 6023 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 6028 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 6030 | CLA  | C6-C7-C8-C9     |
| 22  | d     | 6005 | CLA  | C6-C7-C8-C9     |
| 22  | h     | 6017 | CLA  | C11-C12-C13-C14 |
| 22  | h     | 6017 | CLA  | C14-C13-C15-C16 |
| 23  | A     | 1038 | PHO  | C14-C13-C15-C16 |
| 23  | a     | 6038 | PHO  | C14-C13-C15-C16 |
| 23  | A     | 1038 | PHO  | C15-C16-C17-C18 |
| 23  | a     | 6038 | PHO  | C15-C16-C17-C18 |
| 22  | B     | 1011 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1021 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6011 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6021 | CLA  | C4B-C3B-CAB-CBB |
| 29  | C     | 1055 | DGD  | C2D-C1D-O3G-C3G |
| 29  | c     | 6055 | DGD  | C2D-C1D-O3G-C3G |
| 22  | A     | 1003 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1007 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1011 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1012 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1012 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1016 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1018 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1018 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1019 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1021 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1021 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1023 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1025 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 1030 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 1032 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 1036 | CLA  | C11-C12-C13-C15 |
| 22  | D     | 1005 | CLA  | C11-C12-C13-C15 |
| 22  | H     | 1017 | CLA  | C6-C7-C8-C10    |
| 22  | H     | 1017 | CLA  | C12-C13-C15-C16 |
| 22  | K     | 1034 | CLA  | C6-C7-C8-C10    |
| 22  | a     | 6003 | CLA  | C12-C13-C15-C16 |
| 22  | a     | 6007 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6011 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 6012 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6012 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 6016 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6018 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6018 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6019 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6021 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 6021 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6023 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6025 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6030 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 6036 | CLA  | C11-C12-C13-C15 |
| 22  | d     | 6005 | CLA  | C11-C12-C13-C15 |
| 22  | h     | 6017 | CLA  | C6-C7-C8-C10    |
| 22  | h     | 6017 | CLA  | C12-C13-C15-C16 |
| 22  | k     | 6034 | CLA  | C6-C7-C8-C10    |
| 23  | A     | 1038 | PHO  | C6-C7-C8-C10    |
| 23  | D     | 1039 | PHO  | C11-C10-C8-C7   |
| 23  | a     | 6038 | PHO  | C6-C7-C8-C10    |
| 23  | d     | 6039 | PHO  | C11-C10-C8-C7   |
| 28  | D     | 1059 | MGE  | CDB-CEB-CFB-CGB |
| 28  | d     | 6059 | MGE  | CDB-CEB-CFB-CGB |
| 29  | C     | 1055 | DGD  | C9B-CAB-CBB-CCB |
| 29  | c     | 6055 | DGD  | C9B-CAB-CBB-CCB |
| 22  | A     | 1003 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1022 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 1035 | CLA  | C4-C3-C5-C6     |
| 22  | H     | 1017 | CLA  | C3A-C2A-CAA-CBA |
| 22  | a     | 6003 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6022 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 6035 | CLA  | C4-C3-C5-C6     |
| 22  | h     | 6017 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | D     | 1039 | PHO  | CBA-CGA-O2A-C1  |
| 23  | d     | 6039 | PHO  | CBA-CGA-O2A-C1  |
| 29  | C     | 1056 | DGD  | C2A-C1A-O1G-C1G |
| 29  | c     | 6056 | DGD  | C2A-C1A-O1G-C1G |
| 29  | B     | 1058 | DGD  | C8A-C9A-CAA-CBA |
| 29  | b     | 6058 | DGD  | C8A-C9A-CAA-CBA |
| 25  | C     | 1054 | BCR  | C13-C14-C15-C16 |
| 25  | c     | 6054 | BCR  | C13-C14-C15-C16 |
| 22  | K     | 1034 | CLA  | C10-C11-C12-C13 |
| 22  | k     | 6034 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1007 | CLA  | C2C-C3C-CAC-CBC |
| 22  | c     | 6035 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1023 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6023 | CLA  | C5-C6-C7-C8     |
| 29  | C     | 1057 | DGD  | C1G-C2G-C3G-O3G |
| 29  | c     | 6057 | DGD  | C1G-C2G-C3G-O3G |
| 22  | C     | 1035 | CLA  | O1D-CGD-O2D-CED |
| 23  | D     | 1039 | PHO  | C1-C2-C3-C4     |
| 23  | d     | 6039 | PHO  | C1-C2-C3-C4     |
| 22  | a     | 6007 | CLA  | C2C-C3C-CAC-CBC |
| 22  | B     | 1018 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 6018 | CLA  | C2-C3-C5-C6     |
| 28  | d     | 6059 | MGE  | C3B-C4B-C5B-C6B |
| 29  | C     | 1055 | DGD  | C3A-C4A-C5A-C6A |
| 28  | D     | 1059 | MGE  | C3B-C4B-C5B-C6B |
| 29  | c     | 6055 | DGD  | C3A-C4A-C5A-C6A |
| 22  | B     | 1014 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6014 | CLA  | C16-C17-C18-C20 |
| 29  | C     | 1057 | DGD  | CAB-CBB-CCB-CDB |
| 29  | c     | 6057 | DGD  | CAB-CBB-CCB-CDB |
| 25  | B     | 1045 | BCR  | C5-C6-C7-C8     |
| 25  | b     | 6045 | BCR  | C5-C6-C7-C8     |
| 26  | A     | 1063 | LHG  | C14-C15-C16-C17 |
| 26  | a     | 6063 | LHG  | C14-C15-C16-C17 |
| 22  | B     | 1016 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1026 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 1026 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6016 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6026 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 6026 | CLA  | C8-C10-C11-C12  |
| 29  | B     | 1058 | DGD  | C9B-CAB-CBB-CCB |
| 28  | D     | 1059 | MGE  | C5B-C6B-C7B-C8B |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | d     | 6059 | MGE  | C5B-C6B-C7B-C8B |
| 29  | b     | 6058 | DGD  | C9B-CAB-CBB-CCB |
| 22  | C     | 1028 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 6028 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1010 | CLA  | C8-C10-C11-C12  |
| 28  | D     | 1059 | MGE  | O1G-C1G-C2G-O2G |
| 28  | d     | 6059 | MGE  | O1G-C1G-C2G-O2G |
| 29  | C     | 1056 | DGD  | O2G-C2G-C3G-O3G |
| 29  | c     | 6056 | DGD  | O2G-C2G-C3G-O3G |
| 24  | A     | 1043 | PQ9  | C12-C11-C2-C1   |
| 24  | a     | 6043 | PQ9  | C12-C11-C2-C1   |
| 22  | b     | 6010 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 1035 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 6035 | CLA  | C2-C3-C5-C6     |
| 23  | D     | 1039 | PHO  | C1-C2-C3-C5     |
| 23  | d     | 6039 | PHO  | C1-C2-C3-C5     |
| 28  | B     | 1060 | MGE  | CAA-CBA-CCA-CDA |
| 22  | C     | 1026 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 1032 | CLA  | C11-C12-C13-C14 |
| 22  | D     | 1008 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 6026 | CLA  | C14-C13-C15-C16 |
| 22  | d     | 6008 | CLA  | C11-C10-C8-C9   |
| 28  | b     | 6060 | MGE  | CAA-CBA-CCA-CDA |
| 25  | B     | 1045 | BCR  | C6-C7-C8-C9     |
| 25  | T     | 6046 | BCR  | C6-C7-C8-C9     |
| 25  | b     | 6045 | BCR  | C6-C7-C8-C9     |
| 25  | t     | 1046 | BCR  | C6-C7-C8-C9     |
| 29  | B     | 1058 | DGD  | C1B-C2B-C3B-C4B |
| 29  | b     | 6058 | DGD  | C1B-C2B-C3B-C4B |
| 25  | k     | 6052 | BCR  | C14-C15-C16-C17 |
| 22  | B     | 1012 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1023 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1025 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6011 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6012 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6023 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 6025 | CLA  | C16-C17-C18-C20 |
| 28  | B     | 1060 | MGE  | C2A-C3A-C4A-C5A |
| 28  | b     | 6060 | MGE  | C2A-C3A-C4A-C5A |
| 24  | A     | 1043 | PQ9  | C18-C20-C21-C22 |
| 24  | a     | 6043 | PQ9  | C18-C20-C21-C22 |
| 22  | B     | 1013 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | b     | 6013 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1011 | CLA  | C16-C17-C18-C20 |
| 22  | D     | 1005 | CLA  | C16-C17-C18-C20 |
| 22  | d     | 6005 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1003 | CLA  | C13-C15-C16-C17 |
| 22  | a     | 6003 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1007 | CLA  | C15-C16-C17-C18 |
| 22  | a     | 6007 | CLA  | C15-C16-C17-C18 |
| 28  | D     | 1059 | MGE  | CCB-CDB-CEB-CFB |
| 28  | d     | 6059 | MGE  | CCB-CDB-CEB-CFB |
| 25  | T     | 6046 | BCR  | C16-C17-C18-C36 |
| 25  | T     | 6046 | BCR  | C20-C21-C22-C37 |
| 25  | t     | 1046 | BCR  | C16-C17-C18-C36 |
| 25  | t     | 1046 | BCR  | C20-C21-C22-C37 |
| 22  | B     | 1023 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6023 | CLA  | O1A-CGA-O2A-C1  |
| 22  | D     | 1005 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1019 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 6019 | CLA  | C8-C10-C11-C12  |
| 28  | B     | 1060 | MGE  | C9A-CAA-CBA-CCA |
| 22  | B     | 1009 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1023 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1024 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 1026 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 1026 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 1026 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 1029 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 1030 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1035 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6009 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 6023 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6024 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6026 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 6026 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 6026 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6029 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 6030 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6032 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 6035 | CLA  | C11-C12-C13-C15 |
| 23  | D     | 1039 | PHO  | C11-C12-C13-C15 |
| 23  | d     | 6039 | PHO  | C11-C12-C13-C15 |
| 28  | b     | 6060 | MGE  | C9A-CAA-CBA-CCA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 1028 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 1037 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6028 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6037 | CLA  | C10-C11-C12-C13 |
| 25  | B     | 1045 | BCR  | C17-C18-C19-C20 |
| 25  | D     | 1050 | BCR  | C7-C8-C9-C10    |
| 25  | b     | 6045 | BCR  | C17-C18-C19-C20 |
| 25  | d     | 6050 | BCR  | C7-C8-C9-C10    |
| 22  | d     | 6005 | CLA  | CBA-CGA-O2A-C1  |
| 28  | D     | 1059 | MGE  | C2G-C3G-O3G-C1D |
| 28  | L     | 1061 | MGE  | C2G-C3G-O3G-C1D |
| 28  | d     | 6059 | MGE  | C2G-C3G-O3G-C1D |
| 28  | l     | 6061 | MGE  | C2G-C3G-O3G-C1D |
| 23  | D     | 1039 | PHO  | C16-C17-C18-C20 |
| 23  | d     | 6039 | PHO  | C16-C17-C18-C20 |
| 23  | D     | 1039 | PHO  | O1A-CGA-O2A-C1  |
| 23  | d     | 6039 | PHO  | O1A-CGA-O2A-C1  |
| 28  | D     | 1062 | MGE  | C3G-C2G-O2G-C1B |
| 28  | d     | 6062 | MGE  | C3G-C2G-O2G-C1B |
| 29  | c     | 6056 | DGD  | O1A-C1A-O1G-C1G |
| 22  | A     | 1003 | CLA  | C16-C17-C18-C20 |
| 22  | a     | 6003 | CLA  | C16-C17-C18-C20 |
| 29  | C     | 1056 | DGD  | O1A-C1A-O1G-C1G |
| 22  | C     | 1029 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 6029 | CLA  | C10-C11-C12-C13 |
| 25  | T     | 6046 | BCR  | C20-C21-C22-C23 |
| 25  | t     | 1046 | BCR  | C20-C21-C22-C23 |
| 26  | a     | 6063 | LHG  | C11-C10-C9-C8   |
| 28  | b     | 6060 | MGE  | CDB-CEB-CFB-CGB |
| 26  | A     | 1063 | LHG  | C11-C10-C9-C8   |
| 24  | A     | 1043 | PQ9  | C23-C25-C26-C27 |
| 26  | A     | 1063 | LHG  | C4-C5-C6-O8     |
| 26  | a     | 6063 | LHG  | C4-C5-C6-O8     |
| 29  | B     | 1058 | DGD  | C1G-C2G-C3G-O3G |
| 29  | C     | 1056 | DGD  | C1G-C2G-C3G-O3G |
| 29  | b     | 6058 | DGD  | C1G-C2G-C3G-O3G |
| 29  | c     | 6056 | DGD  | C1G-C2G-C3G-O3G |
| 28  | B     | 1060 | MGE  | CDB-CEB-CFB-CGB |
| 28  | d     | 6059 | MGE  | C1A-C2A-C3A-C4A |
| 22  | B     | 1013 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 6013 | CLA  | C2-C3-C5-C6     |
| 28  | D     | 1059 | MGE  | C1A-C2A-C3A-C4A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | A     | 1043 | PQ9  | C12-C11-C2-C3   |
| 24  | a     | 6043 | PQ9  | C12-C11-C2-C3   |
| 29  | C     | 1057 | DGD  | C7A-C8A-C9A-CAA |
| 22  | B     | 1013 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1020 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 6013 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6020 | CLA  | C15-C16-C17-C18 |
| 29  | c     | 6057 | DGD  | C7A-C8A-C9A-CAA |
| 28  | D     | 1059 | MGE  | O2G-C2G-C3G-O3G |
| 28  | L     | 1061 | MGE  | O1G-C1G-C2G-O2G |
| 28  | d     | 6059 | MGE  | O2G-C2G-C3G-O3G |
| 28  | l     | 6061 | MGE  | O1G-C1G-C2G-O2G |
| 29  | B     | 1058 | DGD  | O2G-C2G-C3G-O3G |
| 29  | C     | 1055 | DGD  | O2G-C2G-C3G-O3G |
| 29  | b     | 6058 | DGD  | O2G-C2G-C3G-O3G |
| 29  | c     | 6055 | DGD  | O2G-C2G-C3G-O3G |
| 22  | B     | 1024 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6024 | CLA  | C14-C13-C15-C16 |
| 22  | K     | 1034 | CLA  | C5-C6-C7-C8     |
| 22  | k     | 6034 | CLA  | C5-C6-C7-C8     |
| 22  | a     | 6006 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1006 | CLA  | O1D-CGD-O2D-CED |
| 29  | C     | 1057 | DGD  | C9B-CAB-CBB-CCB |
| 29  | c     | 6057 | DGD  | C9B-CAB-CBB-CCB |
| 22  | B     | 1012 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 1035 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6012 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 6035 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 1027 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 6027 | CLA  | C2A-CAA-CBA-CGA |
| 28  | L     | 1061 | MGE  | CAB-CBB-CCB-CDB |
| 28  | l     | 6061 | MGE  | CAB-CBB-CCB-CDB |
| 22  | B     | 1023 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6023 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6009 | CLA  | C5-C6-C7-C8     |
| 25  | C     | 1052 | BCR  | C14-C15-C16-C17 |
| 22  | C     | 1033 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1021 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6021 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6033 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1009 | CLA  | C5-C6-C7-C8     |
| 24  | a     | 6043 | PQ9  | C23-C25-C26-C27 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1010 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1022 | CLA  | C4B-C3B-CAB-CBB |
| 22  | D     | 1005 | CLA  | C4B-C3B-CAB-CBB |
| 22  | H     | 1017 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6010 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 6022 | CLA  | C4B-C3B-CAB-CBB |
| 22  | d     | 6005 | CLA  | C4B-C3B-CAB-CBB |
| 22  | h     | 6017 | CLA  | C1A-C2A-CAA-CBA |
| 24  | A     | 1043 | PQ9  | C39-C38-C40-C41 |
| 24  | a     | 6043 | PQ9  | C39-C38-C40-C41 |
| 23  | D     | 1039 | PHO  | C16-C17-C18-C19 |
| 23  | d     | 6039 | PHO  | C16-C17-C18-C19 |
| 29  | b     | 6058 | DGD  | C8B-C9B-CAB-CBB |
| 29  | C     | 1055 | DGD  | CAB-CBB-CCB-CDB |
| 29  | c     | 6055 | DGD  | CAB-CBB-CCB-CDB |
| 24  | a     | 6043 | PQ9  | C40-C41-C42-C43 |
| 22  | A     | 1006 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1006 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1013 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1018 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1021 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 1025 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 1029 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1031 | CLA  | C6-C7-C8-C10    |
| 22  | a     | 6006 | CLA  | C11-C10-C8-C7   |
| 22  | a     | 6006 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6013 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 6018 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 6021 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 6025 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 6029 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6031 | CLA  | C6-C7-C8-C10    |
| 22  | D     | 1004 | CLA  | C2C-C3C-CAC-CBC |
| 28  | L     | 1061 | MGE  | C6A-C7A-C8A-C9A |
| 28  | l     | 6061 | MGE  | C6A-C7A-C8A-C9A |
| 29  | B     | 1058 | DGD  | C8B-C9B-CAB-CBB |
| 28  | D     | 1059 | MGE  | C3A-C4A-C5A-C6A |
| 28  | d     | 6059 | MGE  | C3A-C4A-C5A-C6A |
| 29  | C     | 1057 | DGD  | C4B-C5B-C6B-C7B |
| 29  | c     | 6057 | DGD  | C4B-C5B-C6B-C7B |
| 22  | d     | 6004 | CLA  | C2C-C3C-CAC-CBC |
| 26  | A     | 1063 | LHG  | C2-C3-O3-P      |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | a     | 6063 | LHG  | C2-C3-O3-P      |
| 22  | A     | 1003 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1031 | CLA  | C10-C11-C12-C13 |
| 22  | K     | 1034 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6031 | CLA  | C10-C11-C12-C13 |
| 22  | k     | 6034 | CLA  | C13-C15-C16-C17 |
| 24  | A     | 1043 | PQ9  | C40-C41-C42-C43 |
| 22  | A     | 1003 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 1036 | CLA  | C11-C12-C13-C14 |
| 22  | a     | 6003 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 6032 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 6036 | CLA  | C11-C12-C13-C14 |
| 29  | B     | 1058 | DGD  | C7A-C8A-C9A-CAA |
| 22  | a     | 6003 | CLA  | C16-C17-C18-C19 |
| 29  | b     | 6058 | DGD  | C7A-C8A-C9A-CAA |
| 22  | b     | 6020 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1020 | CLA  | C4C-C3C-CAC-CBC |
| 26  | A     | 1063 | LHG  | O7-C5-C6-O8     |
| 26  | a     | 6063 | LHG  | O7-C5-C6-O8     |
| 28  | B     | 1060 | MGE  | O2G-C2G-C3G-O3G |
| 28  | b     | 6060 | MGE  | O2G-C2G-C3G-O3G |
| 29  | C     | 1056 | DGD  | O1G-C1G-C2G-O2G |
| 29  | c     | 6056 | DGD  | O1G-C1G-C2G-O2G |
| 28  | D     | 1059 | MGE  | O1G-C1G-C2G-C3G |
| 28  | d     | 6059 | MGE  | O1G-C1G-C2G-C3G |
| 28  | D     | 1062 | MGE  | CDB-CEB-CFB-CGB |
| 28  | d     | 6062 | MGE  | C4D-C5D-C6D-O5D |
| 29  | C     | 1055 | DGD  | CDA-CEA-CFA-CGA |
| 29  | c     | 6055 | DGD  | CDA-CEA-CFA-CGA |
| 22  | D     | 1005 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 6018 | CLA  | C8-C10-C11-C12  |
| 22  | d     | 6005 | CLA  | C15-C16-C17-C18 |
| 28  | d     | 6062 | MGE  | CDB-CEB-CFB-CGB |
| 28  | D     | 1062 | MGE  | C4D-C5D-C6D-O5D |
| 22  | C     | 1036 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 6036 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 1018 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1020 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6020 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 1030 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6030 | CLA  | O1A-CGA-O2A-C1  |
| 28  | D     | 1059 | MGE  | C4B-C5B-C6B-C7B |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | d     | 6059 | MGE  | C4B-C5B-C6B-C7B |
| 22  | A     | 1007 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 1018 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 1020 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 1031 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 1032 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 1033 | CLA  | CAD-CBD-CGD-O1D |
| 22  | D     | 1004 | CLA  | CAD-CBD-CGD-O1D |
| 22  | H     | 1017 | CLA  | CHA-CBD-CGD-O1D |
| 22  | K     | 1034 | CLA  | CAD-CBD-CGD-O1D |
| 22  | a     | 6007 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 6018 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 6020 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 6031 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 6032 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 6033 | CLA  | CAD-CBD-CGD-O1D |
| 22  | d     | 6004 | CLA  | CAD-CBD-CGD-O1D |
| 22  | h     | 6017 | CLA  | CHA-CBD-CGD-O1D |
| 22  | k     | 6034 | CLA  | CAD-CBD-CGD-O1D |
| 25  | B     | 1047 | BCR  | C19-C20-C21-C22 |
| 25  | b     | 6047 | BCR  | C19-C20-C21-C22 |
| 26  | a     | 6063 | LHG  | C3-O3-P-O5      |
| 22  | B     | 1022 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 1028 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 6028 | CLA  | C2B-C3B-CAB-CBB |
| 25  | C     | 1052 | BCR  | C1-C6-C7-C8     |
| 25  | k     | 6052 | BCR  | C1-C6-C7-C8     |
| 29  | c     | 6057 | DGD  | C5B-C6B-C7B-C8B |
| 29  | C     | 1057 | DGD  | C5B-C6B-C7B-C8B |
| 29  | C     | 1057 | DGD  | C5A-C6A-C7A-C8A |
| 29  | c     | 6055 | DGD  | C5B-C6B-C7B-C8B |
| 22  | C     | 1026 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6022 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 6026 | CLA  | C16-C17-C18-C20 |
| 29  | C     | 1055 | DGD  | C5B-C6B-C7B-C8B |
| 29  | c     | 6057 | DGD  | C5A-C6A-C7A-C8A |
| 28  | L     | 1061 | MGE  | C2B-C3B-C4B-C5B |
| 28  | l     | 6061 | MGE  | C2B-C3B-C4B-C5B |
| 29  | C     | 1057 | DGD  | C3B-C4B-C5B-C6B |
| 29  | c     | 6057 | DGD  | C3B-C4B-C5B-C6B |
| 25  | Z     | 1053 | BCR  | C18-C19-C20-C21 |
| 25  | z     | 6053 | BCR  | C18-C19-C20-C21 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 1048 | BCR  | C9-C10-C11-C12  |
| 25  | T     | 6048 | BCR  | C9-C10-C11-C12  |
| 22  | A     | 1003 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1006 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1018 | CLA  | C14-C13-C15-C16 |
| 22  | D     | 1004 | CLA  | C14-C13-C15-C16 |
| 22  | a     | 6003 | CLA  | C14-C13-C15-C16 |
| 22  | a     | 6006 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6018 | CLA  | C14-C13-C15-C16 |
| 22  | d     | 6004 | CLA  | C14-C13-C15-C16 |
| 28  | l     | 6061 | MGE  | C4A-C5A-C6A-C7A |
| 22  | D     | 1004 | CLA  | C12-C13-C15-C16 |
| 22  | d     | 6004 | CLA  | C12-C13-C15-C16 |
| 25  | T     | 6046 | BCR  | C16-C17-C18-C19 |
| 25  | t     | 1046 | BCR  | C16-C17-C18-C19 |
| 28  | L     | 1061 | MGE  | C4A-C5A-C6A-C7A |
| 22  | C     | 1032 | CLA  | C4C-C3C-CAC-CBC |
| 22  | c     | 6032 | CLA  | C4C-C3C-CAC-CBC |
| 28  | L     | 1061 | MGE  | C5B-C6B-C7B-C8B |
| 28  | l     | 6061 | MGE  | C5B-C6B-C7B-C8B |
| 25  | B     | 1045 | BCR  | C13-C14-C15-C16 |
| 22  | B     | 1022 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 6022 | CLA  | C16-C17-C18-C19 |
| 29  | C     | 1056 | DGD  | CCA-CDA-CEA-CFA |
| 29  | c     | 6056 | DGD  | CCA-CDA-CEA-CFA |
| 22  | B     | 1022 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 6022 | CLA  | C10-C11-C12-C13 |
| 29  | C     | 1057 | DGD  | C1B-C2B-C3B-C4B |
| 25  | b     | 6045 | BCR  | C13-C14-C15-C16 |
| 29  | c     | 6057 | DGD  | C1B-C2B-C3B-C4B |
| 22  | A     | 1007 | CLA  | C4C-C3C-CAC-CBC |
| 22  | a     | 6007 | CLA  | C4C-C3C-CAC-CBC |
| 22  | B     | 1021 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1029 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6021 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6029 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 1030 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 1037 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 6030 | CLA  | C16-C17-C18-C20 |
| 31  | V     | 1041 | HEM  | CAD-CBD-CGD-O2D |
| 31  | v     | 6041 | HEM  | CAD-CBD-CGD-O2D |
| 22  | B     | 1010 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1016 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6010 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 6016 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6037 | CLA  | C16-C17-C18-C20 |
| 26  | A     | 1063 | LHG  | C34-C35-C36-C37 |
| 29  | C     | 1056 | DGD  | C7B-C8B-C9B-CAB |
| 29  | c     | 6056 | DGD  | C7B-C8B-C9B-CAB |
| 22  | B     | 1014 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1015 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1024 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1031 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 6014 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 6015 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6024 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6031 | CLA  | C12-C13-C15-C16 |
| 26  | a     | 6063 | LHG  | C34-C35-C36-C37 |
| 22  | B     | 1016 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 1033 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 6033 | CLA  | C13-C15-C16-C17 |
| 28  | l     | 6061 | MGE  | O6D-C5D-C6D-O5D |
| 26  | A     | 1063 | LHG  | C12-C13-C14-C15 |
| 22  | b     | 6016 | CLA  | C8-C10-C11-C12  |
| 28  | L     | 1061 | MGE  | O6D-C5D-C6D-O5D |
| 25  | B     | 1048 | BCR  | C20-C21-C22-C37 |
| 25  | K     | 1051 | BCR  | C20-C21-C22-C37 |
| 25  | T     | 6048 | BCR  | C20-C21-C22-C37 |
| 25  | k     | 6051 | BCR  | C20-C21-C22-C37 |
| 22  | B     | 1010 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 6010 | CLA  | C15-C16-C17-C18 |
| 26  | a     | 6063 | LHG  | C12-C13-C14-C15 |
| 22  | B     | 1016 | CLA  | C2-C1-O2A-CGA   |
| 22  | b     | 6016 | CLA  | C2-C1-O2A-CGA   |
| 25  | T     | 6046 | BCR  | C13-C14-C15-C16 |
| 25  | t     | 1046 | BCR  | C13-C14-C15-C16 |
| 31  | V     | 1041 | HEM  | CAD-CBD-CGD-O1D |
| 31  | v     | 6041 | HEM  | CAD-CBD-CGD-O1D |
| 22  | B     | 1009 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1027 | CLA  | C6-C7-C8-C9     |
| 22  | D     | 1005 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6009 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6027 | CLA  | C6-C7-C8-C9     |
| 22  | d     | 6005 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | A     | 1038 | PHO  | C11-C12-C13-C14 |
| 23  | a     | 6038 | PHO  | C11-C12-C13-C14 |
| 28  | L     | 1061 | MGE  | CDB-CEB-CFB-CGB |
| 28  | l     | 6061 | MGE  | CDB-CEB-CFB-CGB |
| 22  | d     | 6005 | CLA  | C13-C15-C16-C17 |
| 22  | D     | 1005 | CLA  | C13-C15-C16-C17 |
| 25  | B     | 1048 | BCR  | C20-C21-C22-C23 |
| 25  | K     | 1051 | BCR  | C20-C21-C22-C23 |
| 25  | T     | 6048 | BCR  | C20-C21-C22-C23 |
| 25  | k     | 6051 | BCR  | C20-C21-C22-C23 |
| 22  | B     | 1010 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1022 | CLA  | C2B-C3B-CAB-CBB |
| 22  | D     | 1005 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6010 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6022 | CLA  | C2B-C3B-CAB-CBB |
| 22  | d     | 6005 | CLA  | C2B-C3B-CAB-CBB |
| 31  | V     | 1041 | HEM  | CAA-CBA-CGA-O1A |
| 31  | v     | 6041 | HEM  | CAA-CBA-CGA-O1A |
| 28  | D     | 1062 | MGE  | C6A-C7A-C8A-C9A |
| 28  | d     | 6062 | MGE  | C6A-C7A-C8A-C9A |
| 22  | B     | 1020 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1022 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 1027 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6022 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 6027 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6020 | CLA  | C16-C17-C18-C20 |
| 29  | C     | 1055 | DGD  | C4B-C5B-C6B-C7B |
| 28  | B     | 1060 | MGE  | C7B-C8B-C9B-CAB |
| 28  | b     | 6060 | MGE  | C7B-C8B-C9B-CAB |
| 29  | c     | 6055 | DGD  | C4B-C5B-C6B-C7B |
| 22  | D     | 1004 | CLA  | C4-C3-C5-C6     |
| 22  | d     | 6004 | CLA  | C4-C3-C5-C6     |
| 28  | D     | 1059 | MGE  | C8A-C9A-CAA-CBA |
| 28  | d     | 6059 | MGE  | C8A-C9A-CAA-CBA |
| 22  | C     | 1036 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 6036 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1007 | CLA  | C11-C10-C8-C9   |
| 22  | a     | 6007 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 1033 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 6033 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1019 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6019 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1011 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 1036 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 6011 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 6036 | CLA  | C4-C3-C5-C6     |
| 24  | A     | 1043 | PQ9  | C37-C38-C40-C41 |
| 24  | a     | 6043 | PQ9  | C37-C38-C40-C41 |
| 22  | B     | 1022 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6022 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 1030 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 6030 | CLA  | C16-C17-C18-C19 |
| 24  | D     | 1042 | PQ9  | C18-C20-C21-C22 |
| 24  | d     | 6042 | PQ9  | C18-C20-C21-C22 |
| 28  | D     | 1062 | MGE  | C1G-C2G-C3G-O3G |
| 28  | d     | 6062 | MGE  | C1G-C2G-C3G-O3G |
| 22  | B     | 1019 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 6019 | CLA  | O1A-CGA-O2A-C1  |
| 29  | B     | 1058 | DGD  | CDA-CEA-CFA-CGA |
| 29  | b     | 6058 | DGD  | CDA-CEA-CFA-CGA |
| 22  | B     | 1021 | CLA  | C8-C10-C11-C12  |
| 29  | B     | 1058 | DGD  | CEB-CFB-CGB-CHB |
| 29  | b     | 6058 | DGD  | CEB-CFB-CGB-CHB |
| 22  | b     | 6021 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1010 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1024 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 6010 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 6024 | CLA  | C4-C3-C5-C6     |
| 31  | V     | 1041 | HEM  | CAA-CBA-CGA-O2A |
| 31  | v     | 6041 | HEM  | CAA-CBA-CGA-O2A |
| 23  | A     | 1038 | PHO  | CHA-CBD-CGD-O1D |
| 23  | A     | 1038 | PHO  | CHA-CBD-CGD-O2D |
| 23  | D     | 1039 | PHO  | CHA-CBD-CGD-O1D |
| 23  | D     | 1039 | PHO  | CHA-CBD-CGD-O2D |
| 23  | a     | 6038 | PHO  | CHA-CBD-CGD-O1D |
| 23  | a     | 6038 | PHO  | CHA-CBD-CGD-O2D |
| 23  | d     | 6039 | PHO  | CHA-CBD-CGD-O1D |
| 23  | d     | 6039 | PHO  | CHA-CBD-CGD-O2D |
| 25  | D     | 1050 | BCR  | C20-C21-C22-C37 |
| 25  | d     | 6050 | BCR  | C20-C21-C22-C37 |
| 28  | B     | 1060 | MGE  | O1G-C1G-C2G-O2G |
| 28  | b     | 6060 | MGE  | O1G-C1G-C2G-O2G |
| 22  | B     | 1011 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 1036 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | D     | 1004 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 6011 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 6036 | CLA  | C2-C3-C5-C6     |
| 22  | d     | 6004 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1015 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 6015 | CLA  | C11-C10-C8-C7   |
| 25  | C     | 1054 | BCR  | C9-C10-C11-C12  |
| 25  | c     | 6054 | BCR  | C9-C10-C11-C12  |
| 23  | A     | 1038 | PHO  | C5-C6-C7-C8     |
| 22  | C     | 1032 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 1036 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 1036 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 6032 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 6036 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 6036 | CLA  | C14-C13-C15-C16 |
| 22  | K     | 1034 | CLA  | C2A-CAA-CBA-CGA |
| 22  | k     | 6034 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1007 | CLA  | C2-C1-O2A-CGA   |
| 22  | a     | 6007 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 1027 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 6027 | CLA  | C5-C6-C7-C8     |
| 23  | a     | 6038 | PHO  | C5-C6-C7-C8     |
| 22  | B     | 1010 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 6010 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1018 | CLA  | C4C-C3C-CAC-CBC |
| 28  | B     | 1060 | MGE  | C6B-C7B-C8B-C9B |
| 28  | b     | 6060 | MGE  | C6B-C7B-C8B-C9B |
| 22  | b     | 6018 | CLA  | C4C-C3C-CAC-CBC |
| 29  | C     | 1056 | DGD  | C4A-C5A-C6A-C7A |
| 29  | b     | 6058 | DGD  | C4A-C5A-C6A-C7A |
| 29  | B     | 1058 | DGD  | C4A-C5A-C6A-C7A |
| 29  | c     | 6056 | DGD  | C4A-C5A-C6A-C7A |
| 22  | B     | 1015 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 6015 | CLA  | C16-C17-C18-C20 |
| 25  | D     | 1050 | BCR  | C20-C21-C22-C23 |
| 25  | d     | 6050 | BCR  | C20-C21-C22-C23 |
| 29  | B     | 1058 | DGD  | CBA-CCA-CDA-CEA |
| 29  | b     | 6058 | DGD  | CBA-CCA-CDA-CEA |
| 29  | c     | 6055 | DGD  | C6A-C7A-C8A-C9A |
| 29  | C     | 1055 | DGD  | C6A-C7A-C8A-C9A |
| 28  | b     | 6060 | MGE  | CAB-CBB-CCB-CDB |
| 28  | B     | 1060 | MGE  | CAB-CBB-CCB-CDB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 29  | c     | 6056 | DGD  | CAB-CBB-CCB-CDB |
| 22  | A     | 1006 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1019 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 1032 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 1036 | CLA  | C11-C10-C8-C7   |
| 22  | K     | 1034 | CLA  | C12-C13-C15-C16 |
| 22  | a     | 6006 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6019 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 6032 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 6036 | CLA  | C11-C10-C8-C7   |
| 22  | k     | 6034 | CLA  | C12-C13-C15-C16 |
| 23  | D     | 1039 | PHO  | C6-C7-C8-C10    |
| 23  | d     | 6039 | PHO  | C6-C7-C8-C10    |
| 29  | C     | 1056 | DGD  | CAB-CBB-CCB-CDB |
| 22  | B     | 1011 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1021 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6011 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 6021 | CLA  | C2B-C3B-CAB-CBB |
| 25  | B     | 1045 | BCR  | C1-C6-C7-C8     |
| 25  | b     | 6045 | BCR  | C1-C6-C7-C8     |
| 22  | K     | 1034 | CLA  | C8-C10-C11-C12  |
| 22  | k     | 6034 | CLA  | C8-C10-C11-C12  |
| 29  | C     | 1055 | DGD  | O2G-C1B-C2B-C3B |
| 29  | c     | 6055 | DGD  | O2G-C1B-C2B-C3B |
| 29  | B     | 1058 | DGD  | C4E-C5E-C6E-O5E |
| 29  | b     | 6058 | DGD  | C4E-C5E-C6E-O5E |
| 22  | B     | 1021 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 1027 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 6018 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 1035 | CLA  | C8-C10-C11-C12  |
| 31  | F     | 1040 | HEM  | CAA-CBA-CGA-O2A |
| 31  | f     | 6040 | HEM  | CAA-CBA-CGA-O2A |
| 22  | c     | 6035 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1018 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 6009 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 6021 | CLA  | CAA-CBA-CGA-O2A |
| 22  | c     | 6027 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1009 | CLA  | CAA-CBA-CGA-O2A |
| 22  | c     | 6029 | CLA  | C5-C6-C7-C8     |
| 28  | B     | 1060 | MGE  | O1G-C1G-C2G-C3G |
| 28  | b     | 6060 | MGE  | O1G-C1G-C2G-C3G |
| 22  | B     | 1010 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1022 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6010 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 6022 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 1029 | CLA  | C5-C6-C7-C8     |
| 28  | B     | 1060 | MGE  | O2G-C1B-C2B-C3B |
| 28  | b     | 6060 | MGE  | O2G-C1B-C2B-C3B |
| 29  | B     | 1058 | DGD  | O2G-C1B-C2B-C3B |
| 28  | b     | 6060 | MGE  | C3B-C4B-C5B-C6B |
| 29  | b     | 6058 | DGD  | O2G-C1B-C2B-C3B |
| 28  | B     | 1060 | MGE  | C3B-C4B-C5B-C6B |
| 22  | C     | 1028 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 1031 | CLA  | C2-C1-O2A-CGA   |
| 22  | c     | 6028 | CLA  | C2-C1-O2A-CGA   |
| 22  | c     | 6031 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1011 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 6011 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1013 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1020 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 1036 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 6013 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 6020 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 6036 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1012 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 6012 | CLA  | C13-C15-C16-C17 |
| 26  | a     | 6063 | LHG  | C11-C12-C13-C14 |
| 26  | A     | 1063 | LHG  | C11-C12-C13-C14 |
| 22  | C     | 1031 | CLA  | CAA-CBA-CGA-O2A |
| 22  | c     | 6031 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1022 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 1028 | CLA  | C2A-CAA-CBA-CGA |
| 22  | D     | 1004 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 6022 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 6028 | CLA  | C2A-CAA-CBA-CGA |
| 22  | d     | 6004 | CLA  | C2A-CAA-CBA-CGA |
| 31  | f     | 6040 | HEM  | CAA-CBA-CGA-O1A |
| 31  | F     | 1040 | HEM  | CAA-CBA-CGA-O1A |
| 31  | F     | 1040 | HEM  | CAD-CBD-CGD-O2D |
| 31  | f     | 6040 | HEM  | CAD-CBD-CGD-O2D |
| 31  | V     | 1041 | HEM  | C3D-CAD-CBD-CGD |
| 31  | v     | 6041 | HEM  | C3D-CAD-CBD-CGD |
| 22  | B     | 1014 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1024 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 1028 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 6014 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 6024 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 6028 | CLA  | C11-C10-C8-C9   |
| 28  | D     | 1059 | MGE  | C2B-C3B-C4B-C5B |
| 28  | d     | 6059 | MGE  | C2B-C3B-C4B-C5B |
| 22  | B     | 1013 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 6013 | CLA  | C10-C11-C12-C13 |
| 24  | D     | 1042 | PQ9  | C14-C13-C15-C16 |
| 24  | d     | 6042 | PQ9  | C14-C13-C15-C16 |
| 22  | K     | 1034 | CLA  | CAA-CBA-CGA-O2A |
| 22  | k     | 6034 | CLA  | CAA-CBA-CGA-O2A |
| 29  | C     | 1055 | DGD  | O1B-C1B-C2B-C3B |
| 29  | c     | 6055 | DGD  | O1B-C1B-C2B-C3B |
| 22  | b     | 6015 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1018 | CLA  | CAA-CBA-CGA-O1A |
| 22  | b     | 6018 | CLA  | CAA-CBA-CGA-O1A |
| 29  | B     | 1058 | DGD  | C5D-C6D-O5D-C1E |
| 29  | b     | 6058 | DGD  | C5D-C6D-O5D-C1E |
| 22  | H     | 1017 | CLA  | CAA-CBA-CGA-O1A |
| 22  | h     | 6017 | CLA  | CAA-CBA-CGA-O1A |
| 28  | B     | 1060 | MGE  | O1B-C1B-C2B-C3B |
| 28  | b     | 6060 | MGE  | O1B-C1B-C2B-C3B |
| 22  | B     | 1015 | CLA  | C8-C10-C11-C12  |
| 28  | L     | 1061 | MGE  | C8A-C9A-CAA-CBA |
| 28  | l     | 6061 | MGE  | C8A-C9A-CAA-CBA |
| 31  | V     | 1041 | HEM  | C2C-C3C-CAC-CBC |
| 22  | A     | 1007 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 1012 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 1030 | CLA  | CAD-CBD-CGD-O2D |
| 22  | a     | 6007 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 6012 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 6030 | CLA  | CAD-CBD-CGD-O2D |
| 22  | a     | 6003 | CLA  | C10-C11-C12-C13 |
| 29  | B     | 1058 | DGD  | O1B-C1B-C2B-C3B |
| 29  | b     | 6058 | DGD  | O1B-C1B-C2B-C3B |
| 22  | c     | 6037 | CLA  | CAA-CBA-CGA-O2A |
| 23  | A     | 1038 | PHO  | CAA-CBA-CGA-O2A |
| 28  | B     | 1060 | MGE  | CCB-CDB-CEB-CFB |
| 28  | b     | 6060 | MGE  | CCB-CDB-CEB-CFB |
| 31  | F     | 1040 | HEM  | CAD-CBD-CGD-O1D |
| 31  | f     | 6040 | HEM  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1003 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 1037 | CLA  | CAA-CBA-CGA-O2A |
| 23  | a     | 6038 | PHO  | CAA-CBA-CGA-O2A |
| 22  | C     | 1025 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 6025 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 1024 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 6024 | CLA  | CBA-CGA-O2A-C1  |

There are no ring outliers.

122 monomers are involved in 4181 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | a     | 6003 | CLA  | 51      | 0            |
| 23  | a     | 6038 | PHO  | 63      | 0            |
| 22  | B     | 1013 | CLA  | 65      | 0            |
| 24  | D     | 1042 | PQ9  | 56      | 0            |
| 22  | c     | 6026 | CLA  | 28      | 0            |
| 22  | A     | 1006 | CLA  | 44      | 0            |
| 29  | c     | 6056 | DGD  | 59      | 0            |
| 22  | b     | 6014 | CLA  | 41      | 0            |
| 31  | v     | 6041 | HEM  | 10      | 0            |
| 25  | t     | 1046 | BCR  | 44      | 0            |
| 22  | a     | 6006 | CLA  | 47      | 0            |
| 23  | A     | 1038 | PHO  | 63      | 0            |
| 22  | D     | 1005 | CLA  | 58      | 0            |
| 28  | D     | 1062 | MGE  | 21      | 0            |
| 25  | b     | 6045 | BCR  | 21      | 0            |
| 25  | k     | 6052 | BCR  | 51      | 0            |
| 22  | B     | 1020 | CLA  | 52      | 0            |
| 22  | D     | 1008 | CLA  | 48      | 0            |
| 22  | B     | 1015 | CLA  | 47      | 0            |
| 22  | C     | 1031 | CLA  | 63      | 0            |
| 22  | B     | 1016 | CLA  | 46      | 0            |
| 22  | C     | 1032 | CLA  | 42      | 0            |
| 22  | k     | 6034 | CLA  | 93      | 0            |
| 25  | C     | 1052 | BCR  | 38      | 0            |
| 22  | B     | 1018 | CLA  | 34      | 0            |
| 22  | B     | 1021 | CLA  | 60      | 0            |
| 26  | A     | 1063 | LHG  | 36      | 0            |
| 22  | b     | 6024 | CLA  | 45      | 0            |
| 22  | b     | 6011 | CLA  | 87      | 0            |
| 22  | d     | 6004 | CLA  | 52      | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | K     | 1051 | BCR  | 27      | 0            |
| 25  | T     | 6048 | BCR  | 23      | 0            |
| 22  | c     | 6030 | CLA  | 37      | 0            |
| 22  | A     | 1003 | CLA  | 51      | 0            |
| 22  | b     | 6019 | CLA  | 37      | 0            |
| 28  | d     | 6062 | MGE  | 21      | 0            |
| 22  | b     | 6012 | CLA  | 61      | 0            |
| 22  | B     | 1014 | CLA  | 44      | 0            |
| 22  | c     | 6028 | CLA  | 37      | 0            |
| 22  | C     | 1033 | CLA  | 66      | 0            |
| 22  | h     | 6017 | CLA  | 47      | 0            |
| 22  | C     | 1027 | CLA  | 35      | 0            |
| 22  | b     | 6010 | CLA  | 37      | 0            |
| 25  | a     | 6044 | BCR  | 26      | 0            |
| 22  | B     | 1023 | CLA  | 68      | 0            |
| 22  | d     | 6008 | CLA  | 46      | 0            |
| 25  | Z     | 1053 | BCR  | 17      | 0            |
| 29  | B     | 1058 | DGD  | 32      | 0            |
| 22  | c     | 6033 | CLA  | 68      | 0            |
| 25  | D     | 1050 | BCR  | 40      | 0            |
| 25  | B     | 1048 | BCR  | 23      | 0            |
| 22  | c     | 6032 | CLA  | 39      | 0            |
| 22  | D     | 1004 | CLA  | 51      | 0            |
| 22  | a     | 6007 | CLA  | 38      | 0            |
| 22  | C     | 1025 | CLA  | 64      | 0            |
| 31  | f     | 6040 | HEM  | 17      | 0            |
| 22  | B     | 1010 | CLA  | 38      | 0            |
| 22  | K     | 1034 | CLA  | 89      | 0            |
| 29  | C     | 1056 | DGD  | 55      | 0            |
| 24  | d     | 6042 | PQ9  | 55      | 0            |
| 22  | c     | 6027 | CLA  | 37      | 0            |
| 22  | b     | 6023 | CLA  | 67      | 0            |
| 22  | C     | 1036 | CLA  | 22      | 0            |
| 22  | C     | 1028 | CLA  | 37      | 0            |
| 22  | b     | 6022 | CLA  | 76      | 0            |
| 22  | d     | 6005 | CLA  | 57      | 0            |
| 22  | B     | 1011 | CLA  | 86      | 0            |
| 22  | C     | 1029 | CLA  | 62      | 0            |
| 25  | A     | 1044 | BCR  | 25      | 0            |
| 22  | C     | 1030 | CLA  | 37      | 0            |
| 22  | C     | 1035 | CLA  | 53      | 0            |
| 25  | b     | 6047 | BCR  | 42      | 0            |

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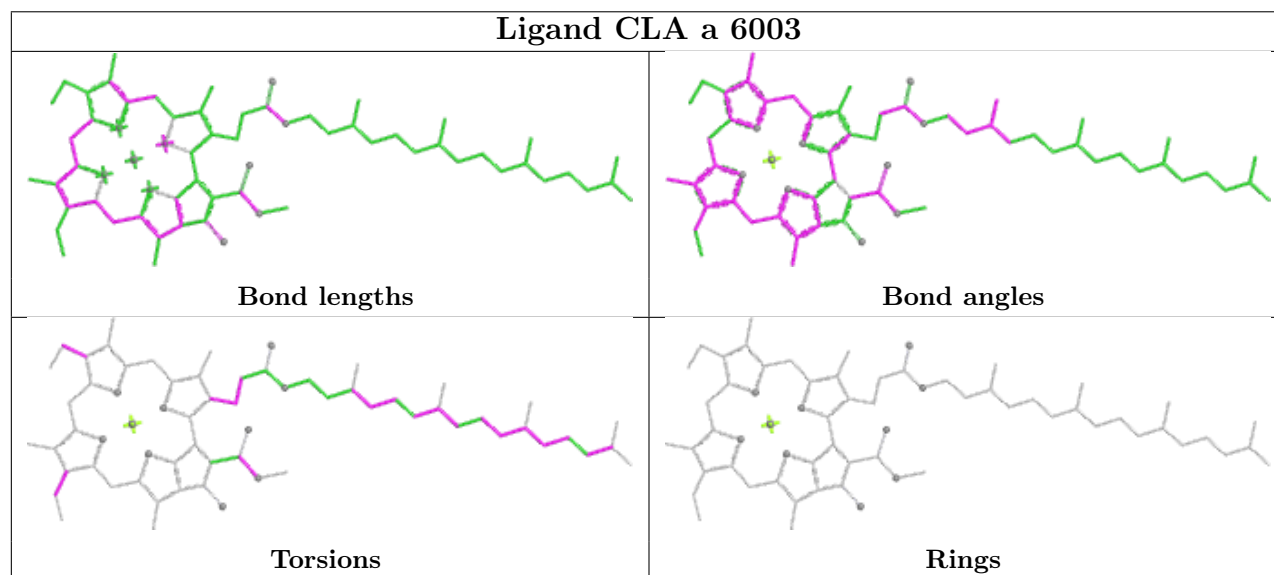
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 23  | d     | 6039 | PHO  | 52      | 0            |
| 22  | c     | 6037 | CLA  | 21      | 0            |
| 22  | c     | 6025 | CLA  | 65      | 0            |
| 26  | a     | 6063 | LHG  | 36      | 0            |
| 25  | k     | 6051 | BCR  | 26      | 0            |
| 31  | V     | 1041 | HEM  | 12      | 0            |
| 22  | b     | 6013 | CLA  | 63      | 0            |
| 25  | B     | 1045 | BCR  | 21      | 0            |
| 22  | b     | 6021 | CLA  | 57      | 0            |
| 22  | b     | 6018 | CLA  | 35      | 0            |
| 22  | A     | 1007 | CLA  | 39      | 0            |
| 22  | B     | 1012 | CLA  | 61      | 0            |
| 22  | b     | 6015 | CLA  | 46      | 0            |
| 22  | C     | 1037 | CLA  | 21      | 0            |
| 22  | B     | 1024 | CLA  | 45      | 0            |
| 28  | b     | 6060 | MGE  | 38      | 0            |
| 22  | B     | 1019 | CLA  | 40      | 0            |
| 25  | B     | 1047 | BCR  | 43      | 0            |
| 29  | c     | 6055 | DGD  | 25      | 0            |
| 25  | T     | 6046 | BCR  | 44      | 0            |
| 22  | b     | 6009 | CLA  | 62      | 0            |
| 25  | h     | 6049 | BCR  | 34      | 0            |
| 25  | H     | 1049 | BCR  | 34      | 0            |
| 28  | L     | 1061 | MGE  | 29      | 0            |
| 29  | c     | 6057 | DGD  | 41      | 0            |
| 28  | B     | 1060 | MGE  | 39      | 0            |
| 22  | c     | 6031 | CLA  | 61      | 0            |
| 25  | c     | 6054 | BCR  | 36      | 0            |
| 25  | C     | 1054 | BCR  | 38      | 0            |
| 29  | b     | 6058 | DGD  | 34      | 0            |
| 22  | H     | 1017 | CLA  | 46      | 0            |
| 29  | C     | 1055 | DGD  | 26      | 0            |
| 22  | b     | 6020 | CLA  | 52      | 0            |
| 28  | d     | 6059 | MGE  | 46      | 0            |
| 22  | c     | 6036 | CLA  | 21      | 0            |
| 22  | b     | 6016 | CLA  | 43      | 0            |
| 28  | D     | 1059 | MGE  | 45      | 0            |
| 25  | z     | 6053 | BCR  | 19      | 0            |
| 28  | l     | 6061 | MGE  | 27      | 0            |
| 29  | C     | 1057 | DGD  | 41      | 0            |
| 24  | A     | 1043 | PQ9  | 36      | 0            |
| 22  | B     | 1009 | CLA  | 59      | 0            |

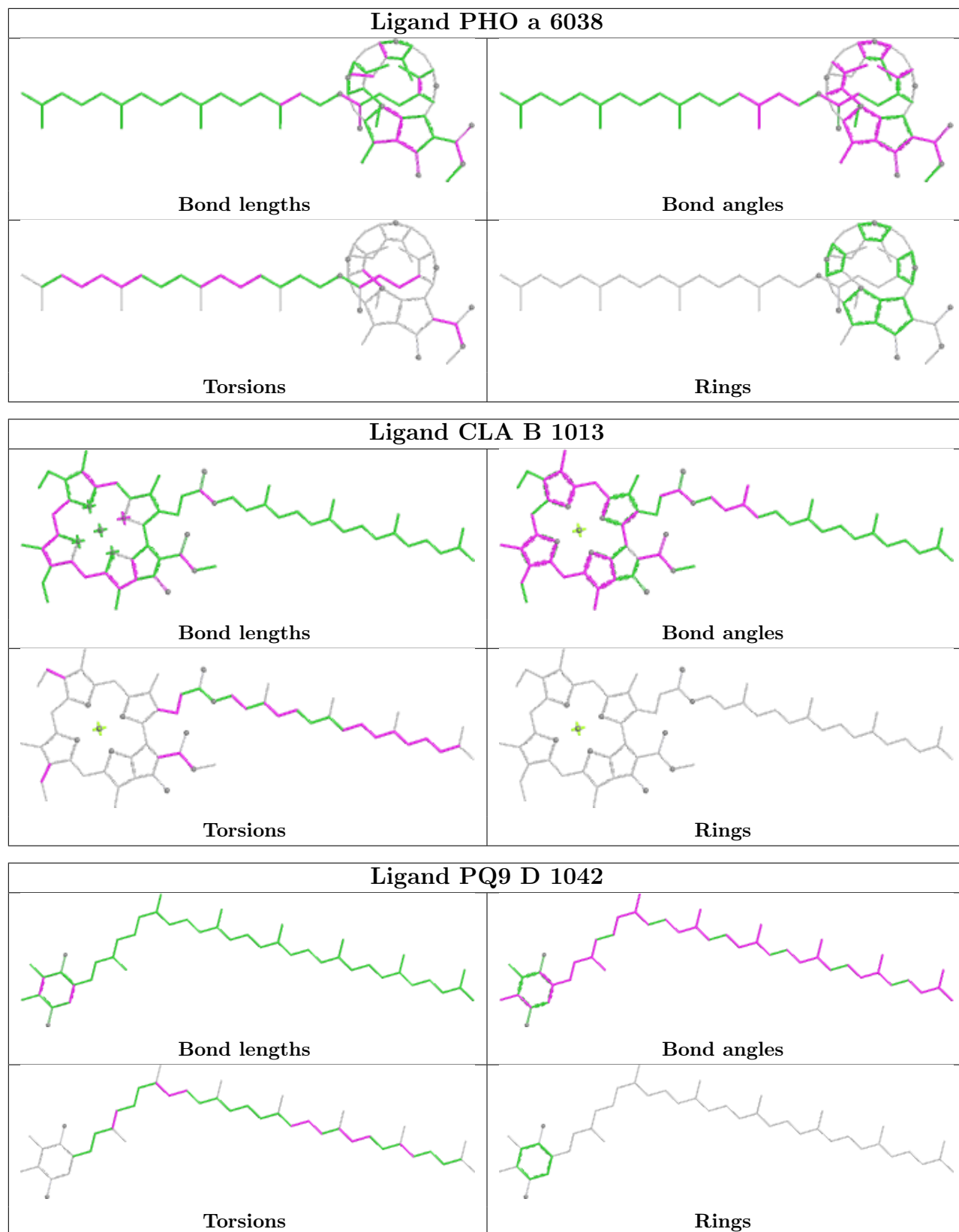
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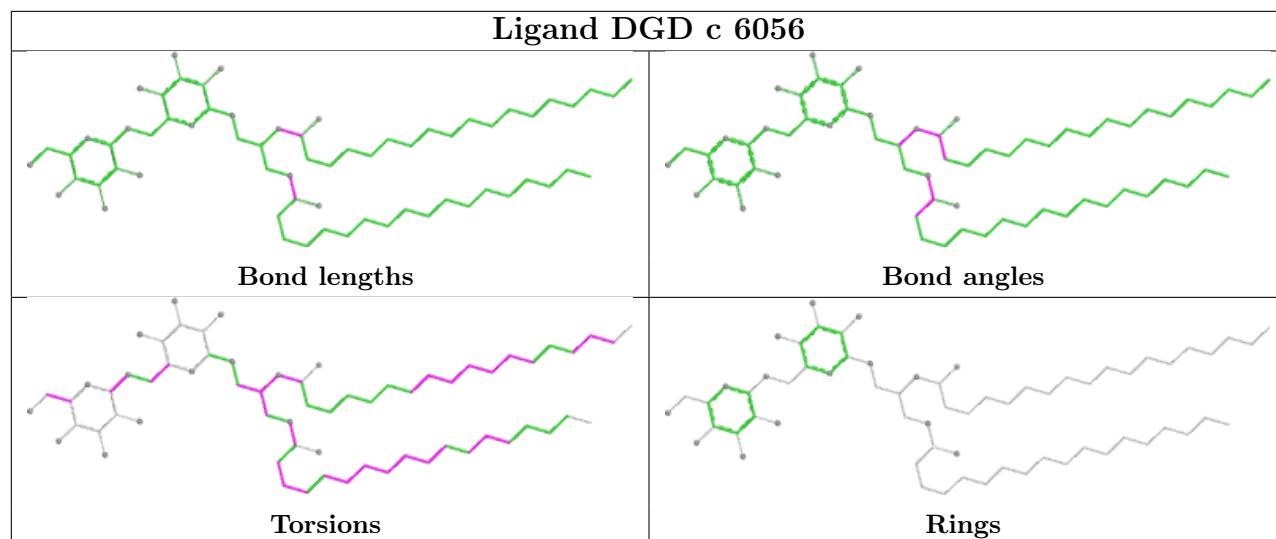
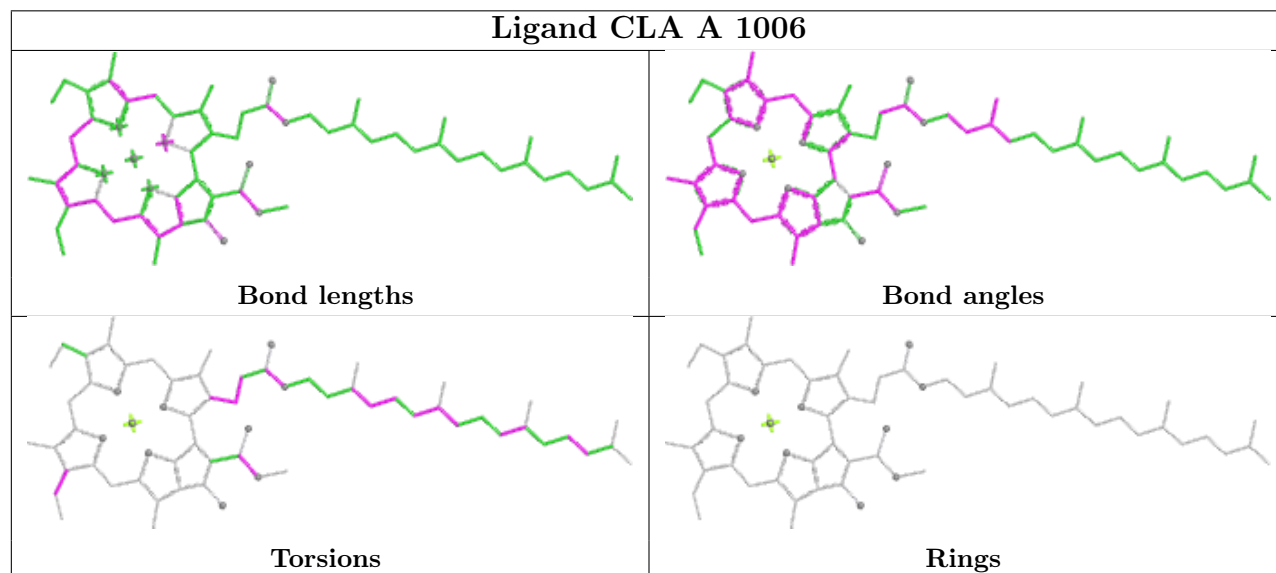
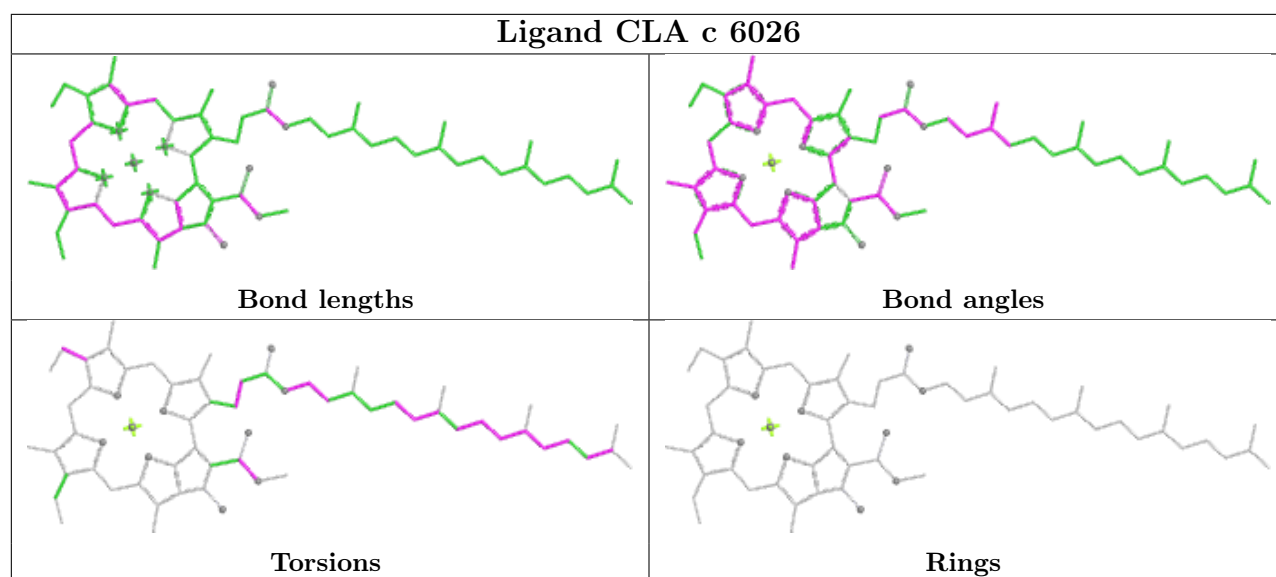
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | d     | 6050 | BCR  | 39      | 0            |
| 22  | B     | 1022 | CLA  | 74      | 0            |
| 31  | F     | 1040 | HEM  | 17      | 0            |
| 22  | C     | 1026 | CLA  | 27      | 0            |
| 22  | c     | 6035 | CLA  | 49      | 0            |
| 23  | D     | 1039 | PHO  | 51      | 0            |
| 24  | a     | 6043 | PQ9  | 35      | 0            |
| 22  | c     | 6029 | CLA  | 59      | 0            |

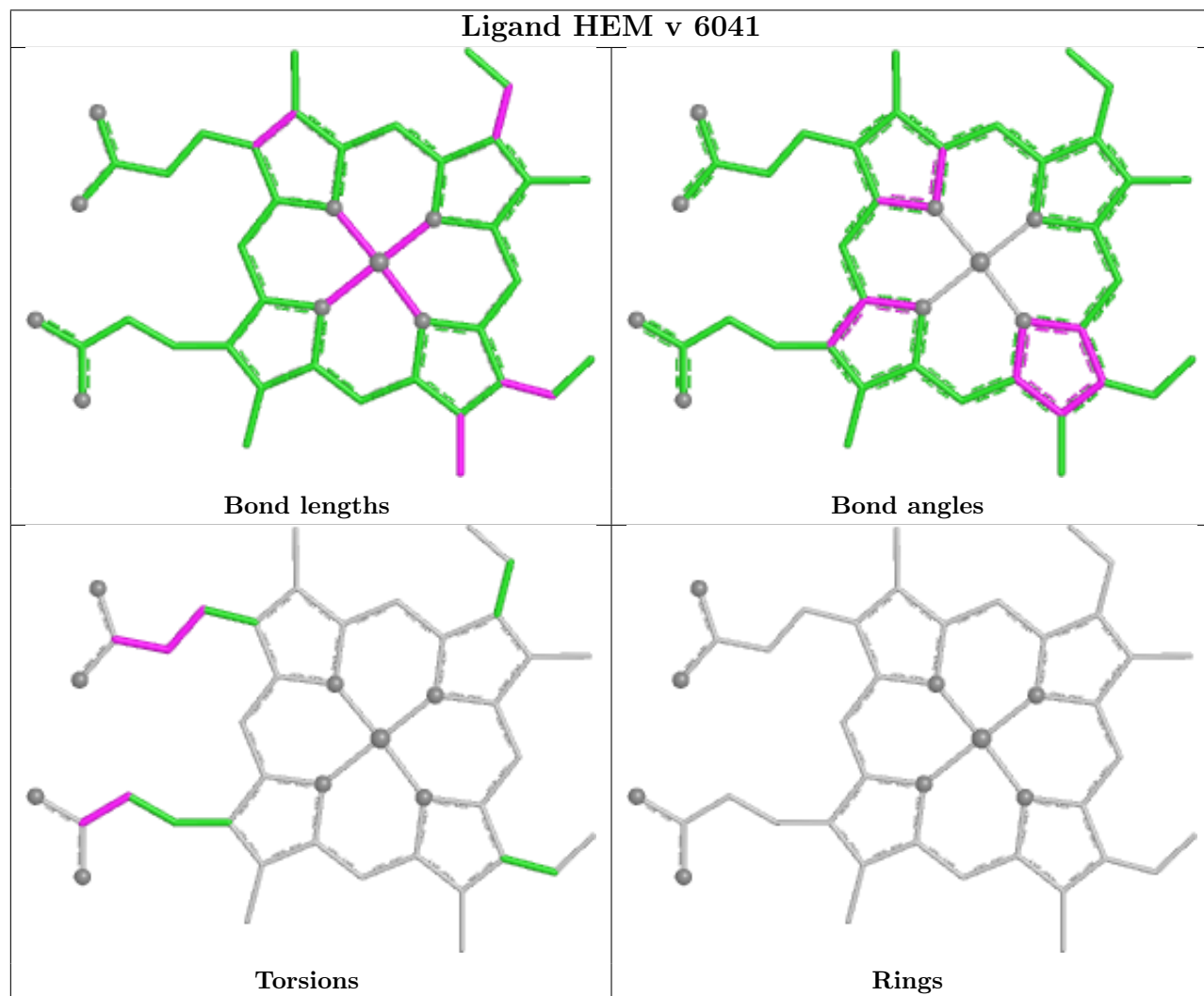
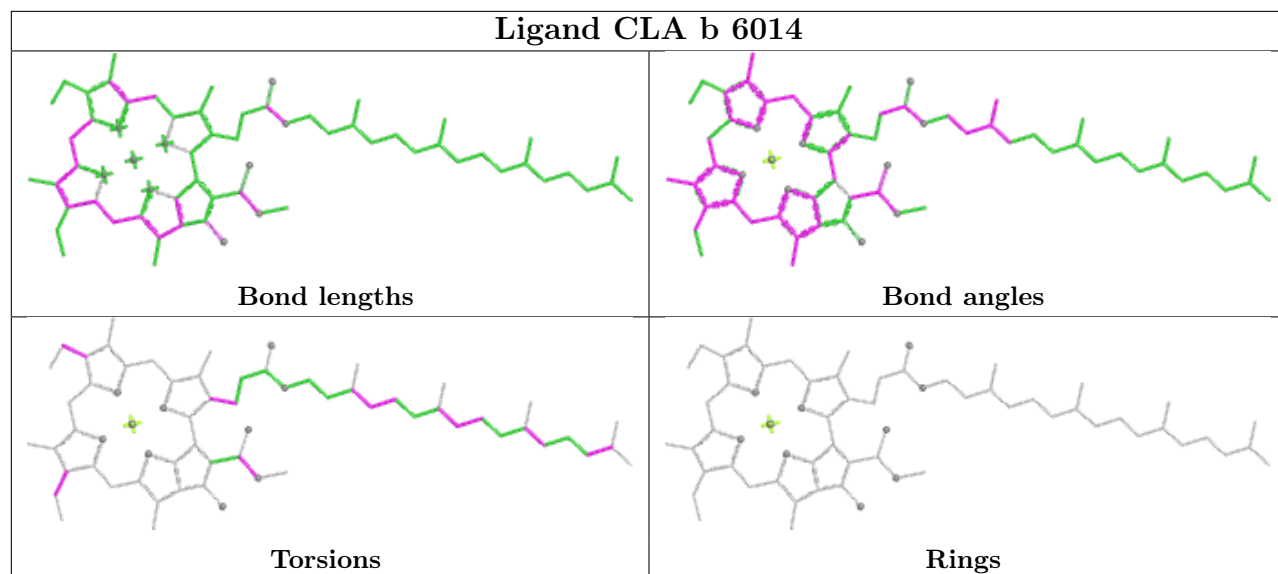
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

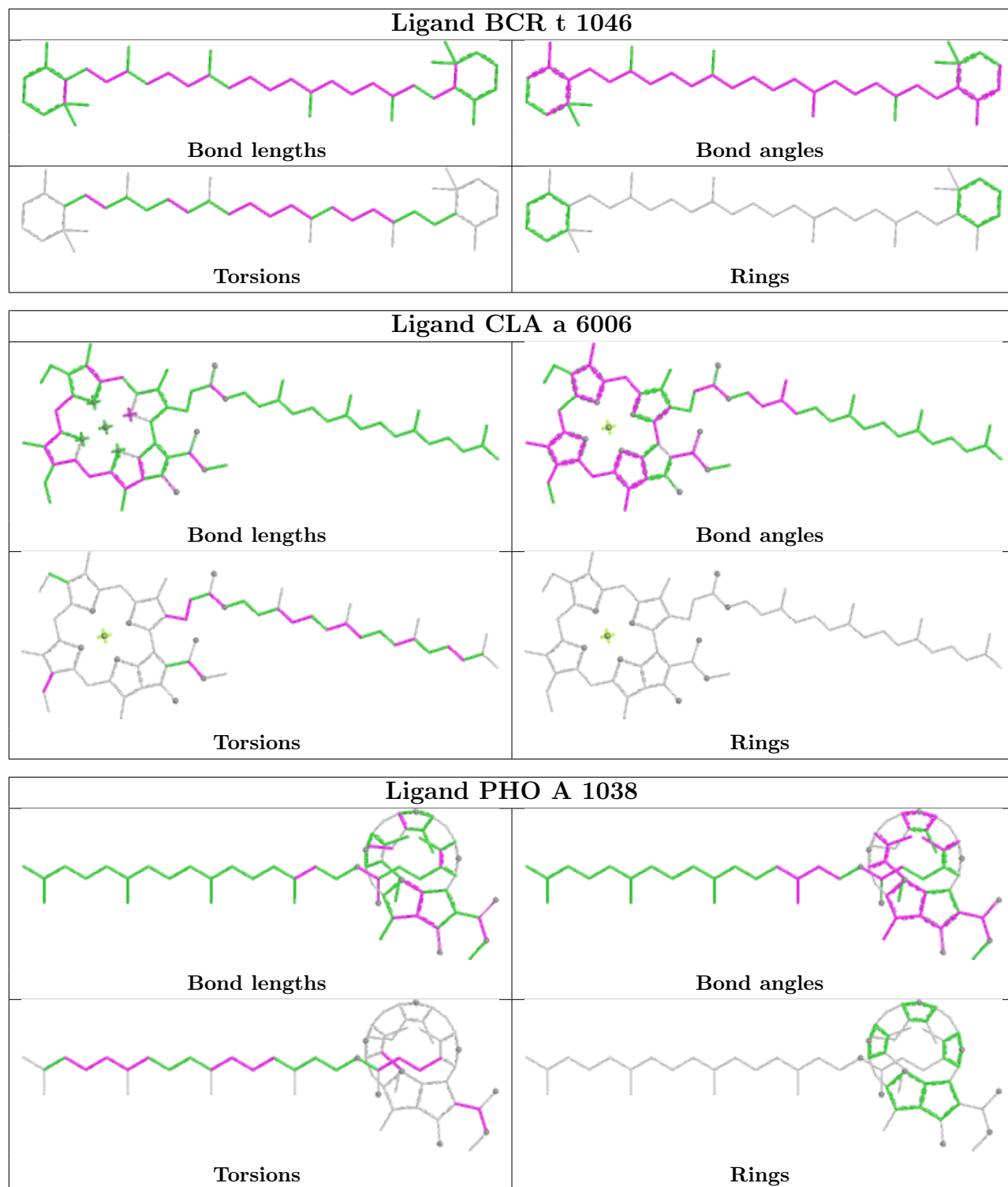


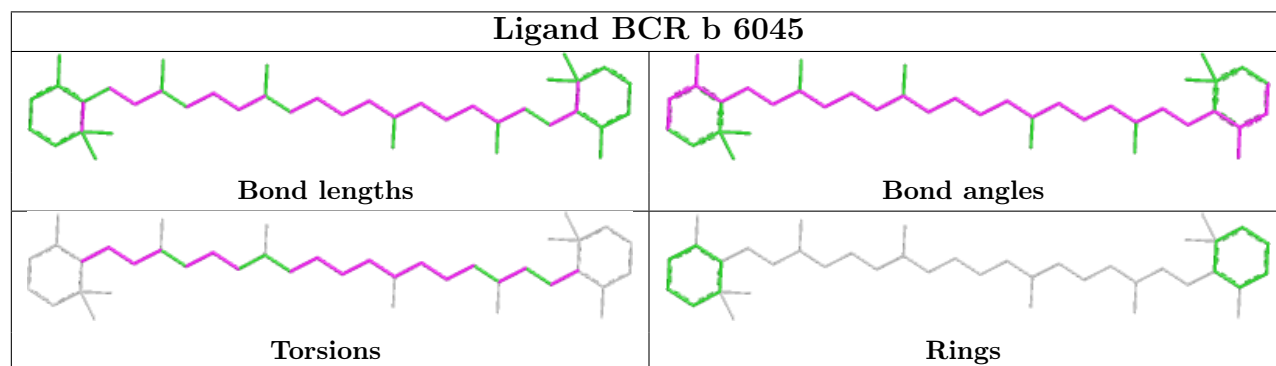
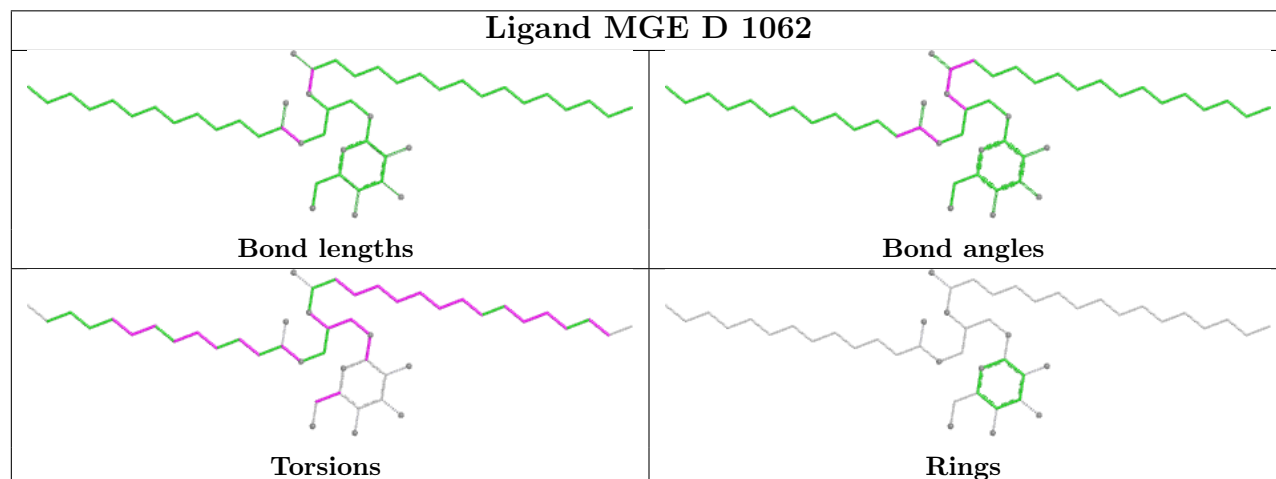
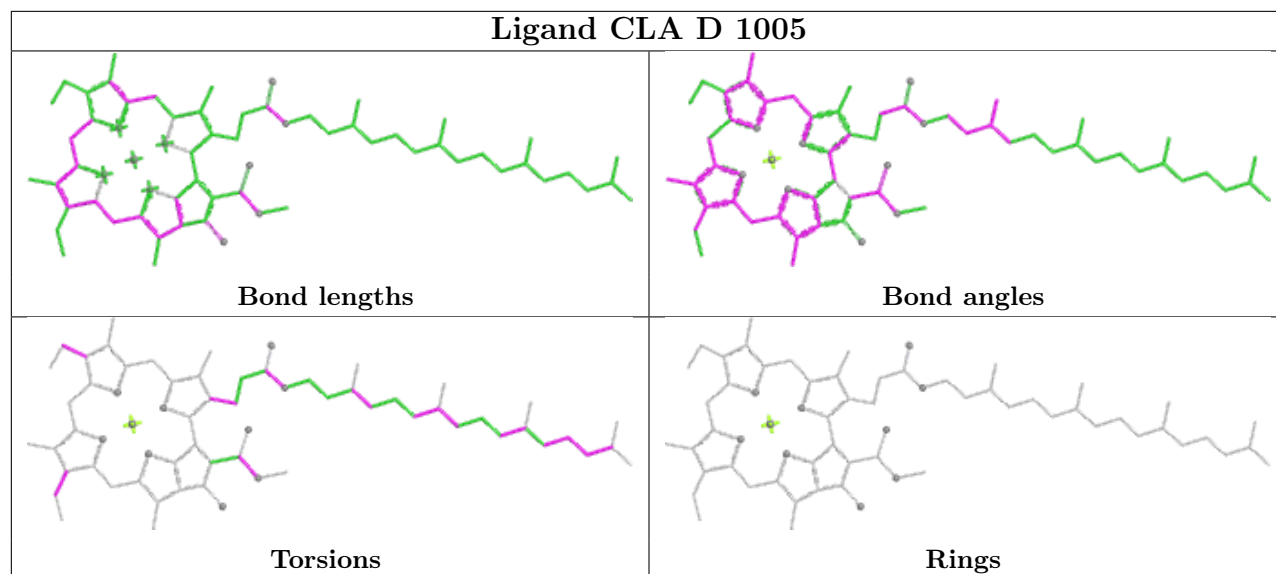


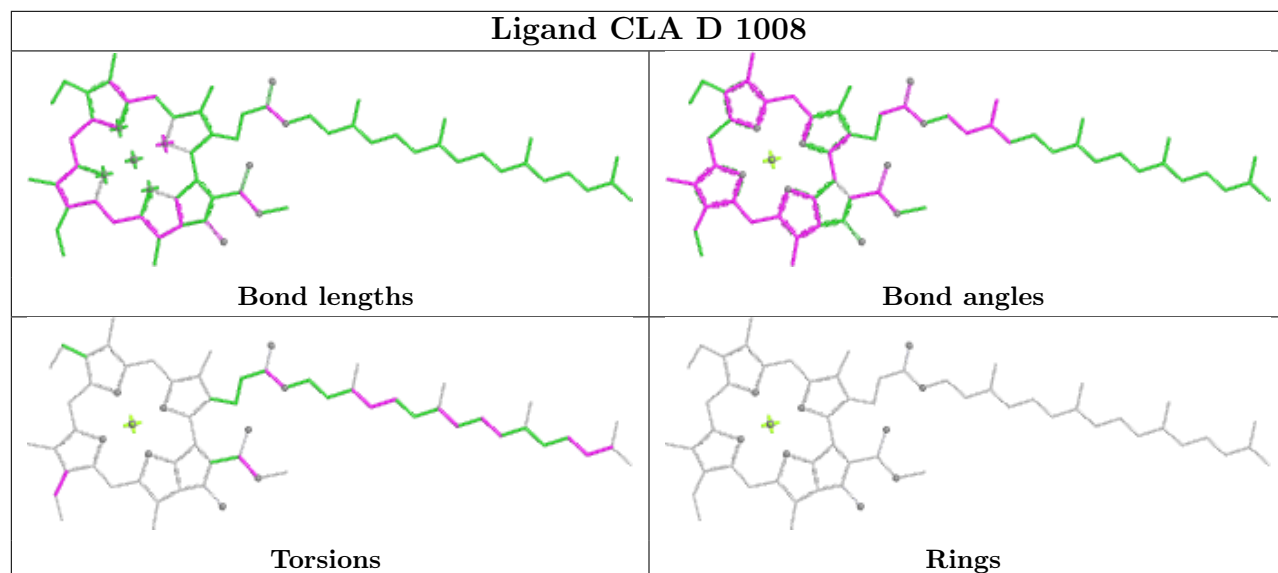
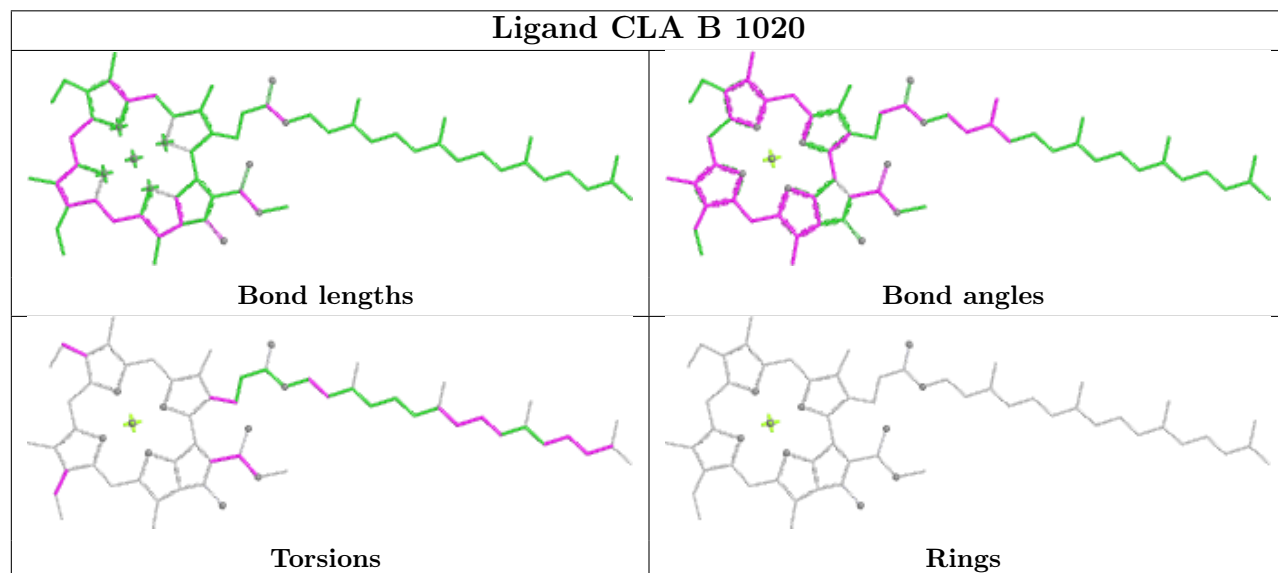
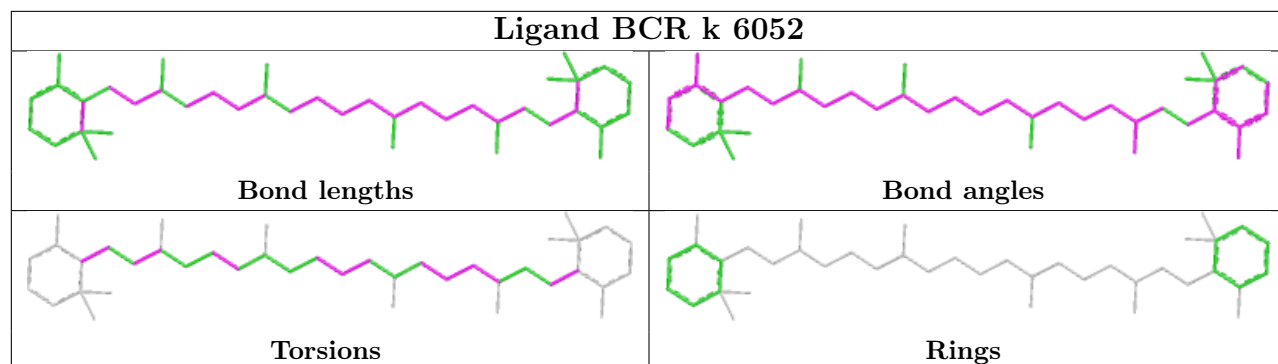




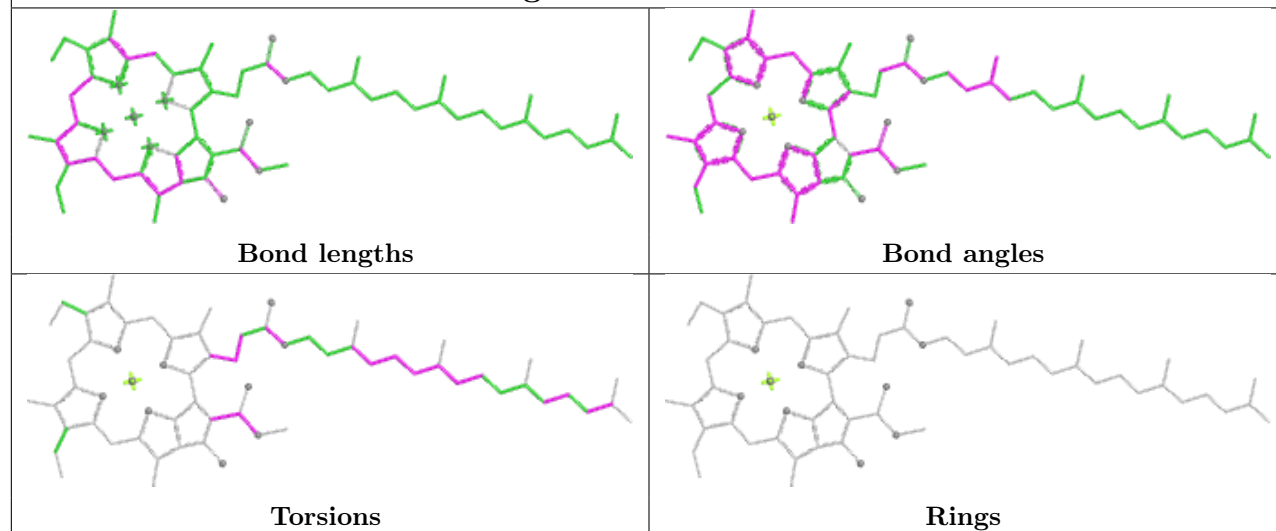




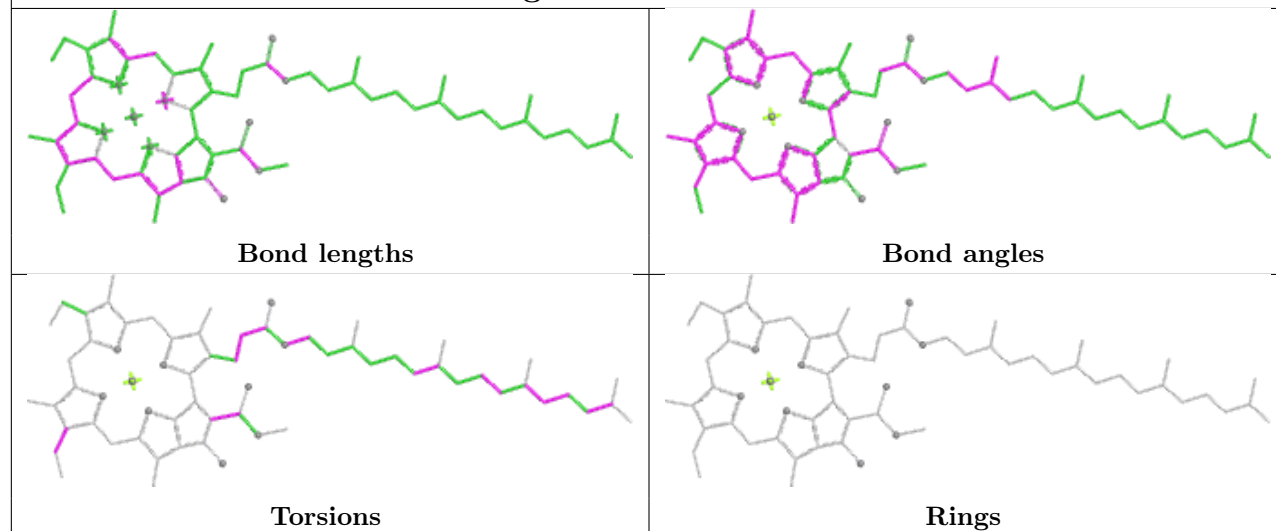




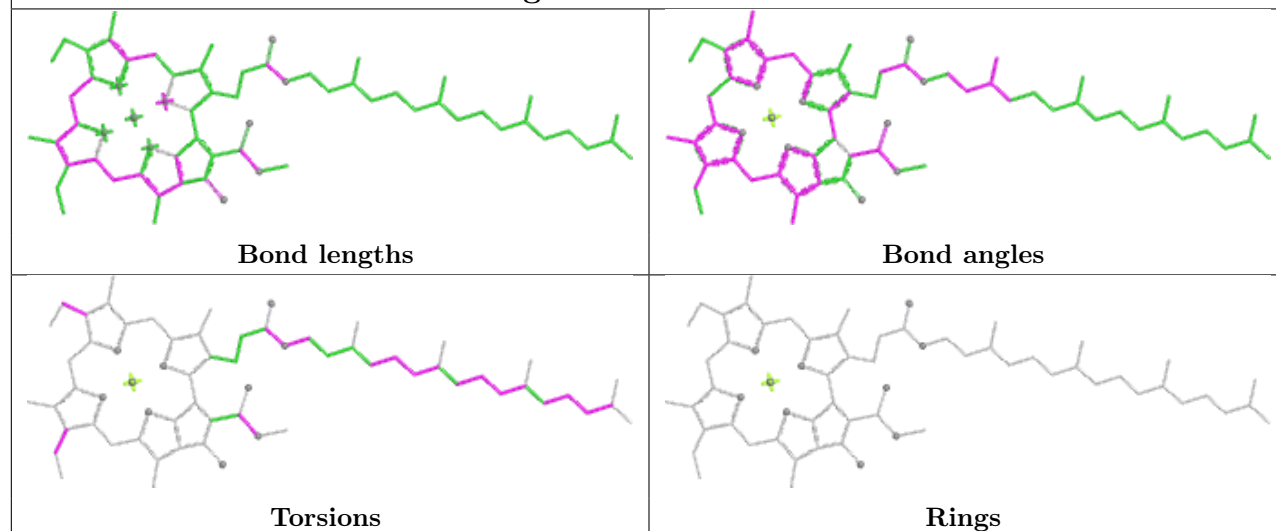
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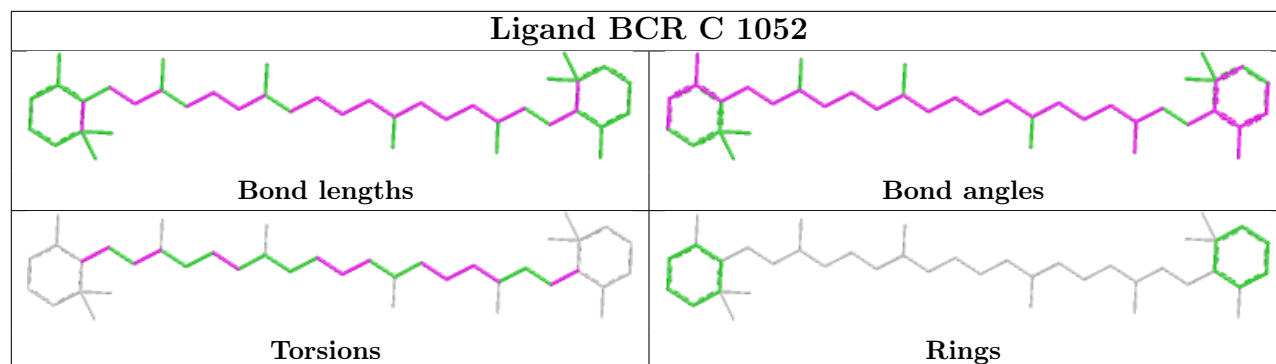
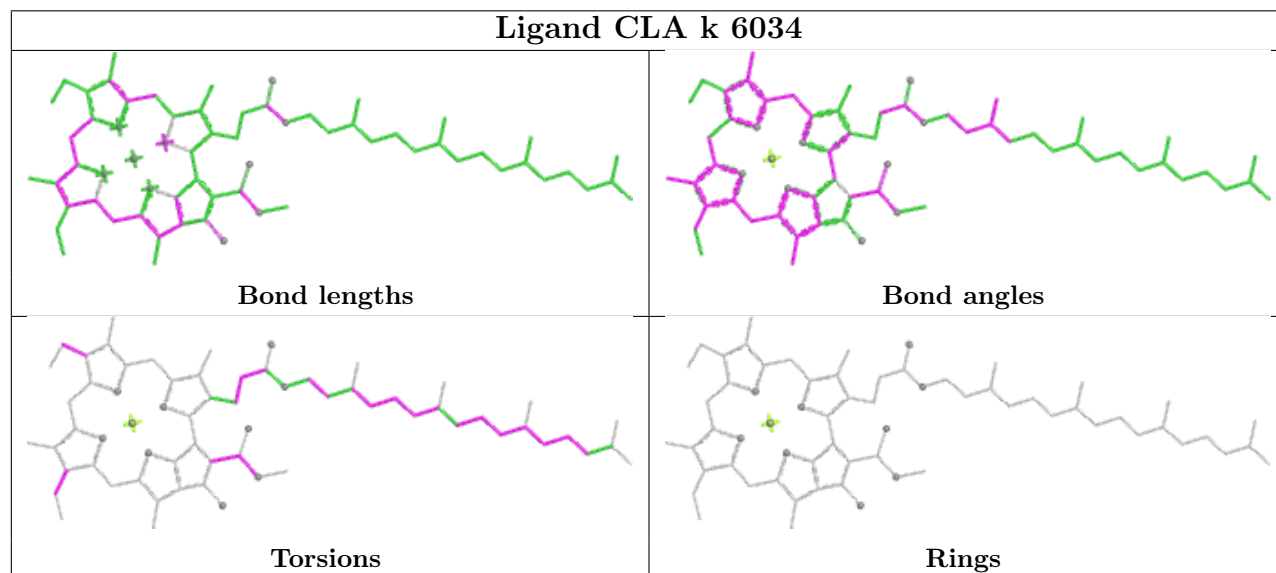
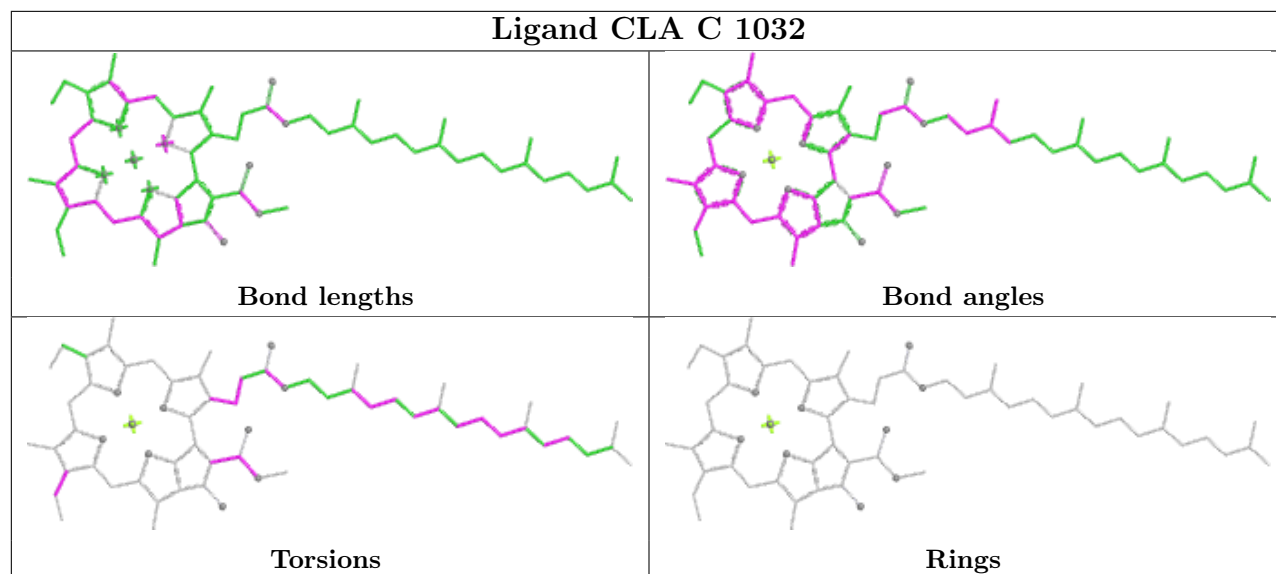


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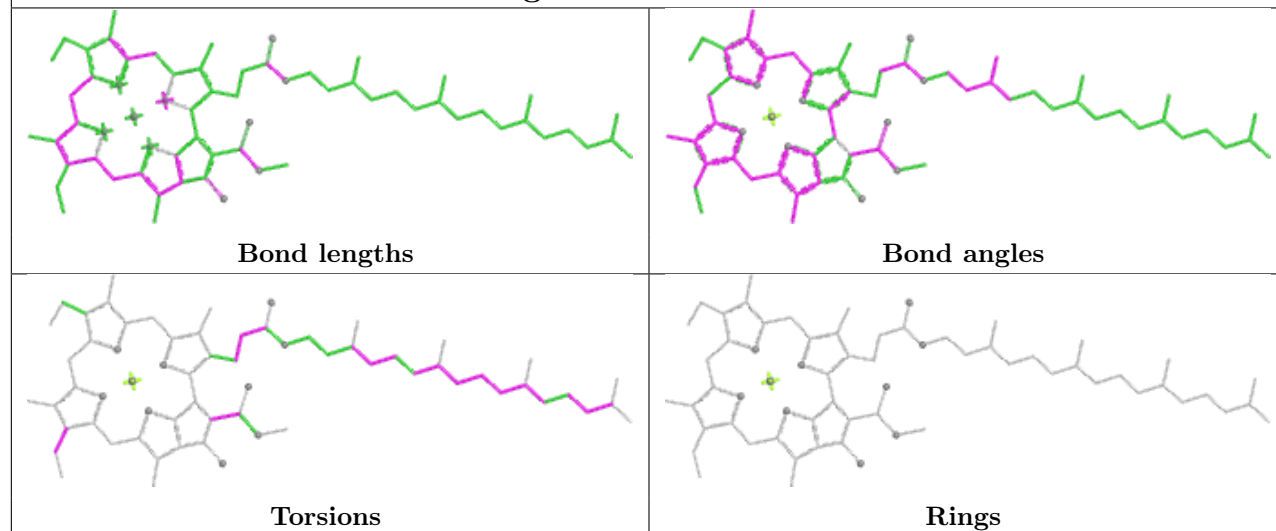
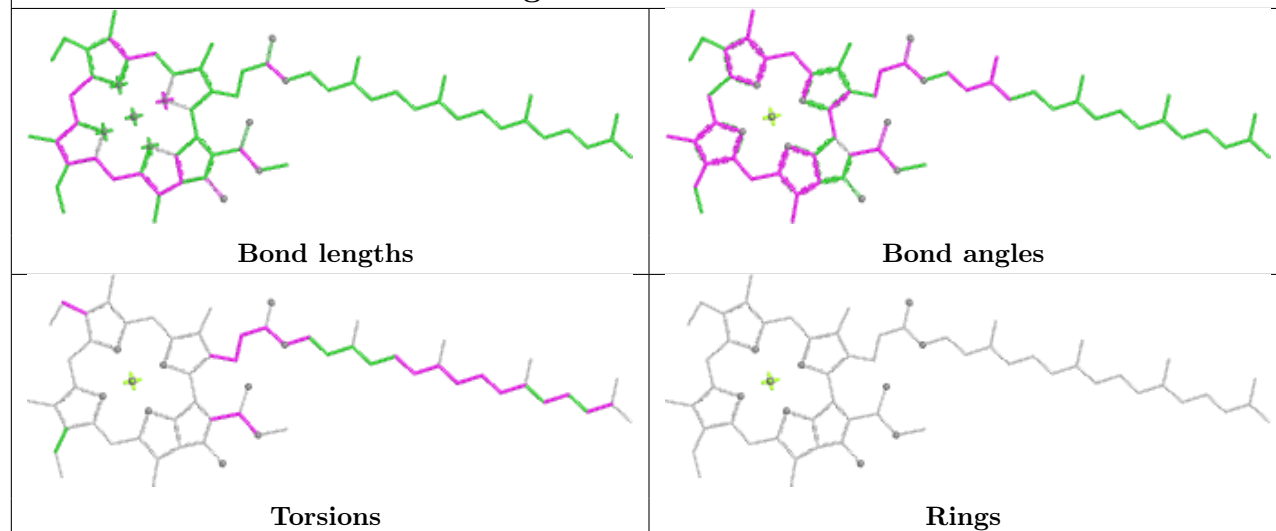


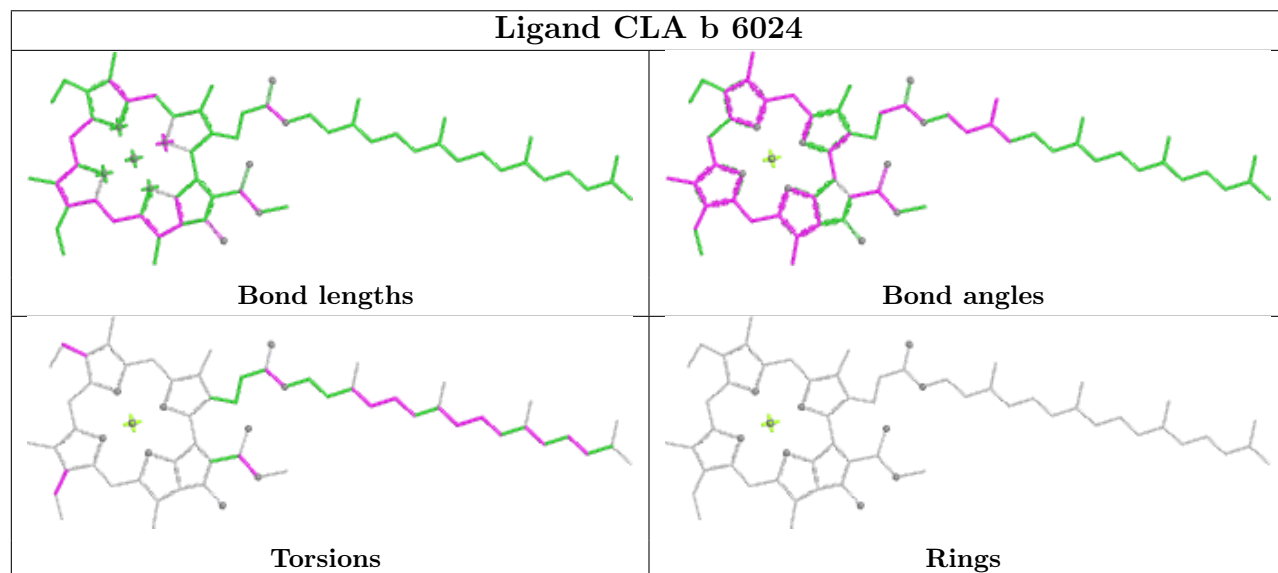
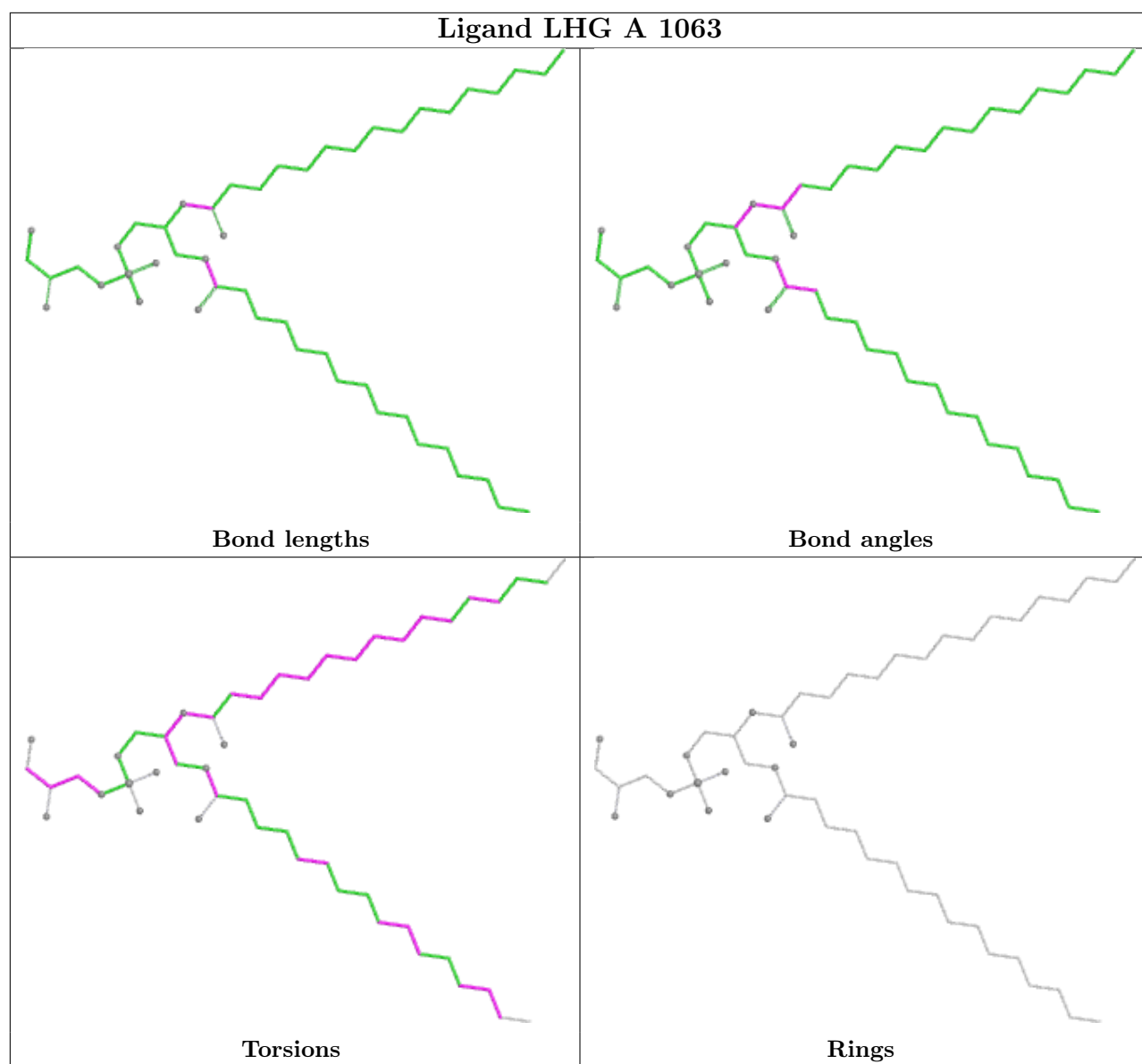
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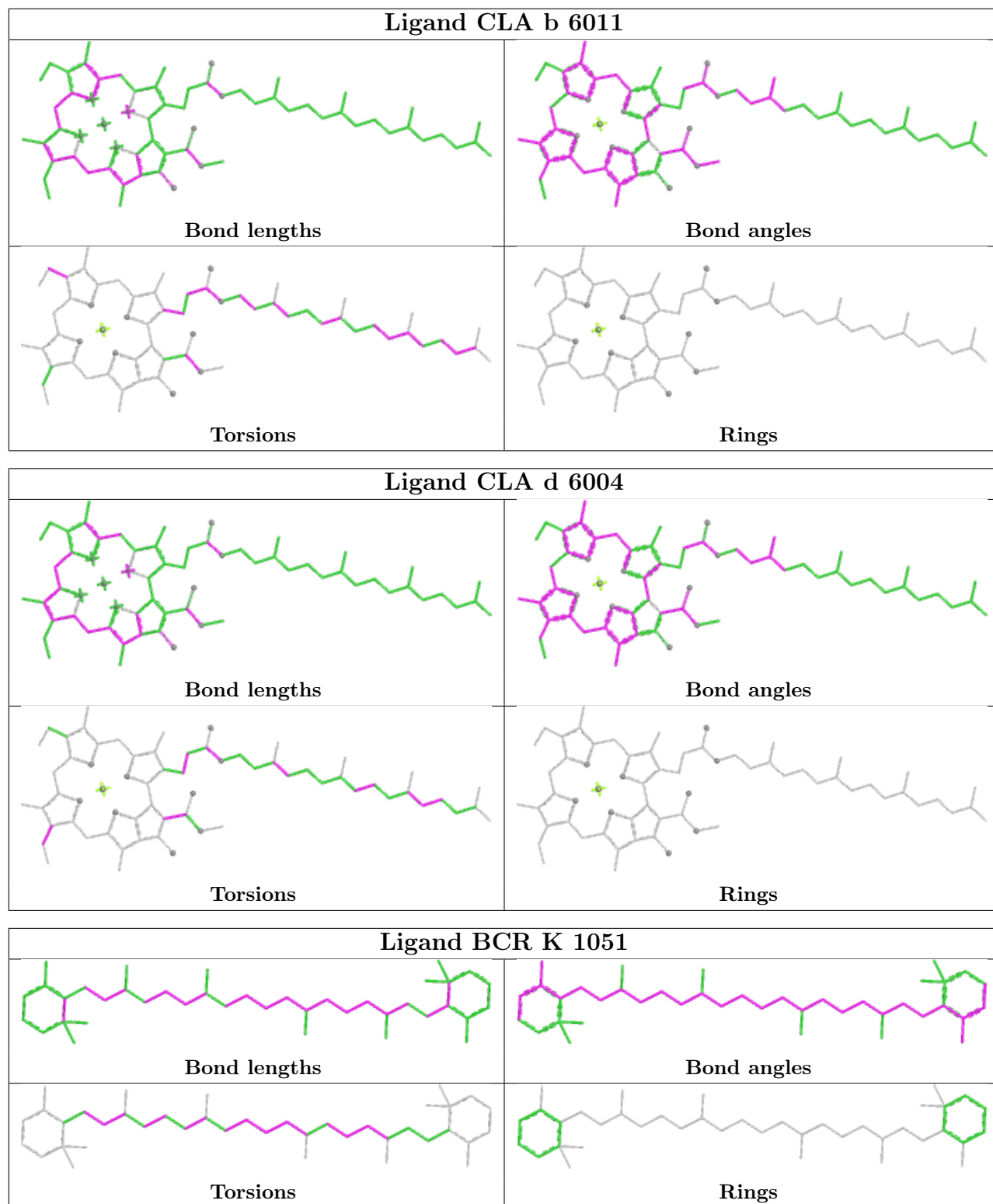




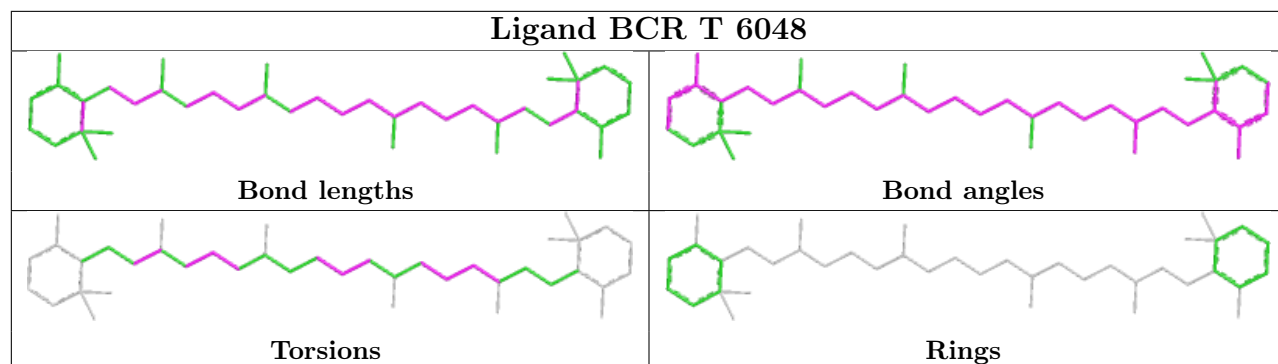


**Ligand CLA B 1018****Ligand CLA B 1021**

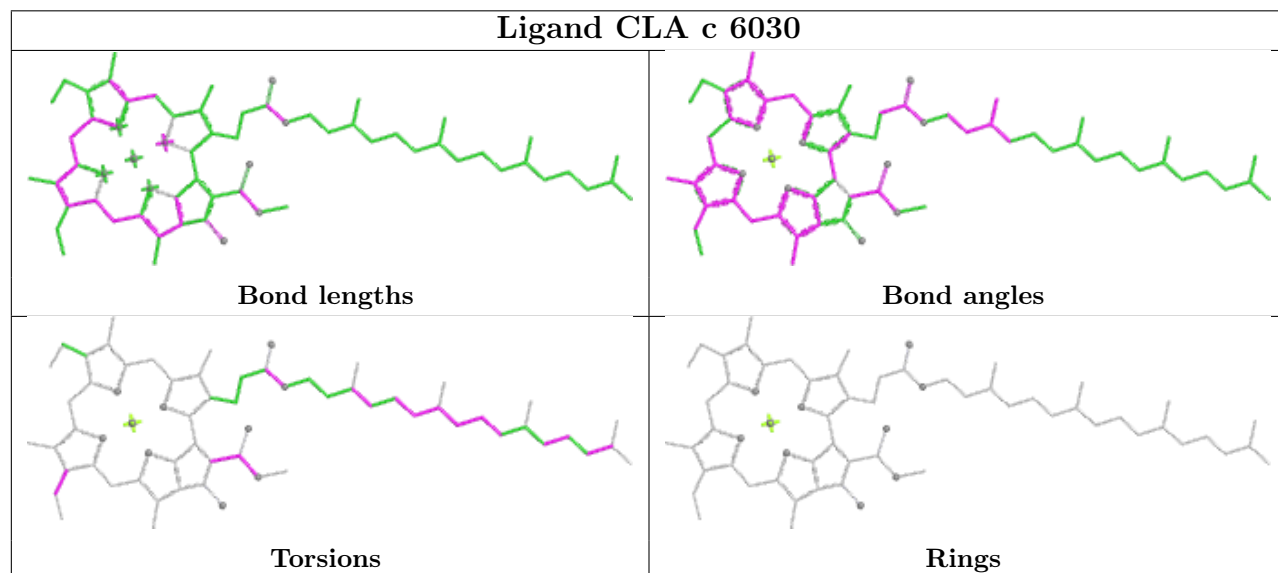




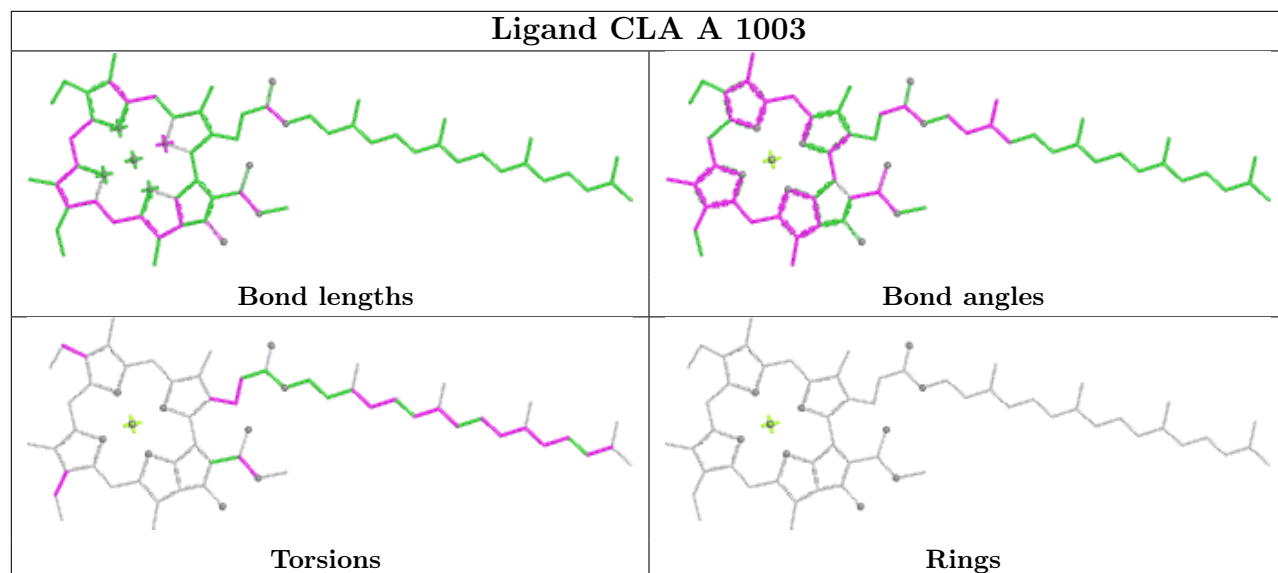
## Ligand BCR T 6048

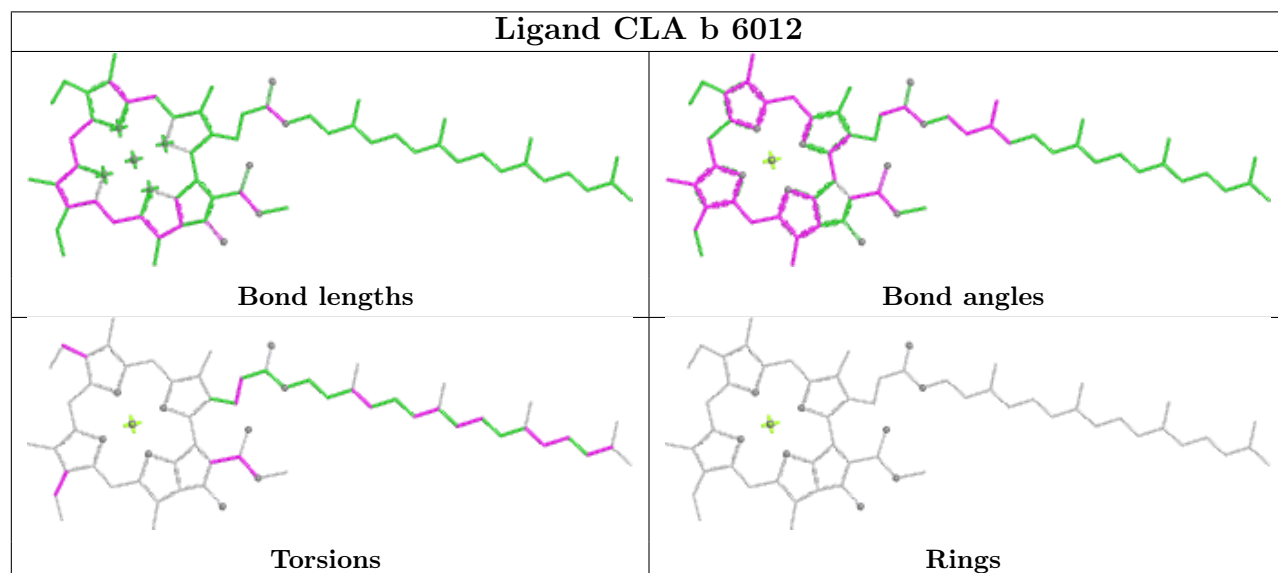
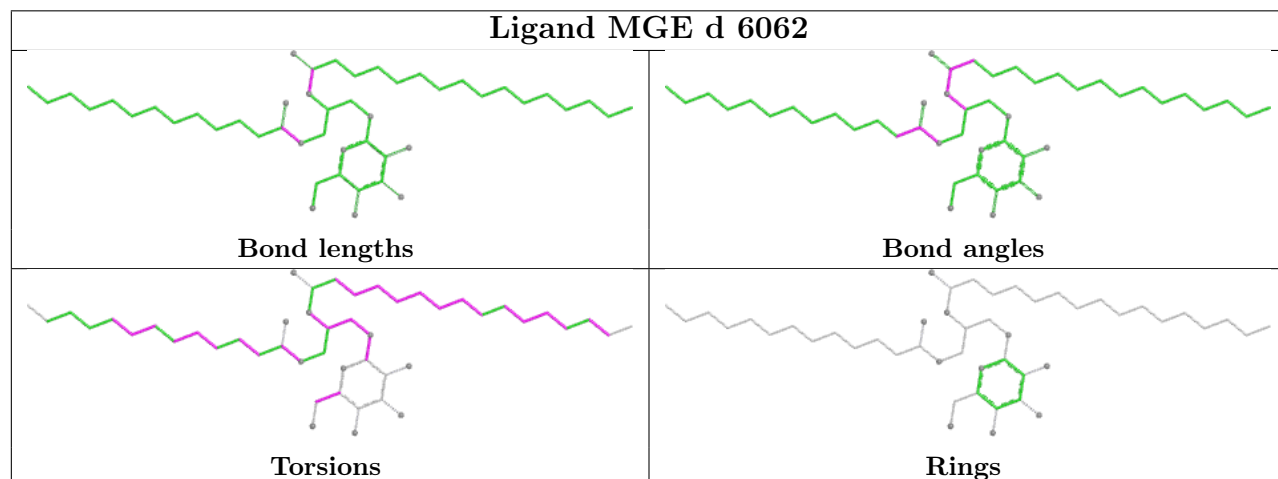
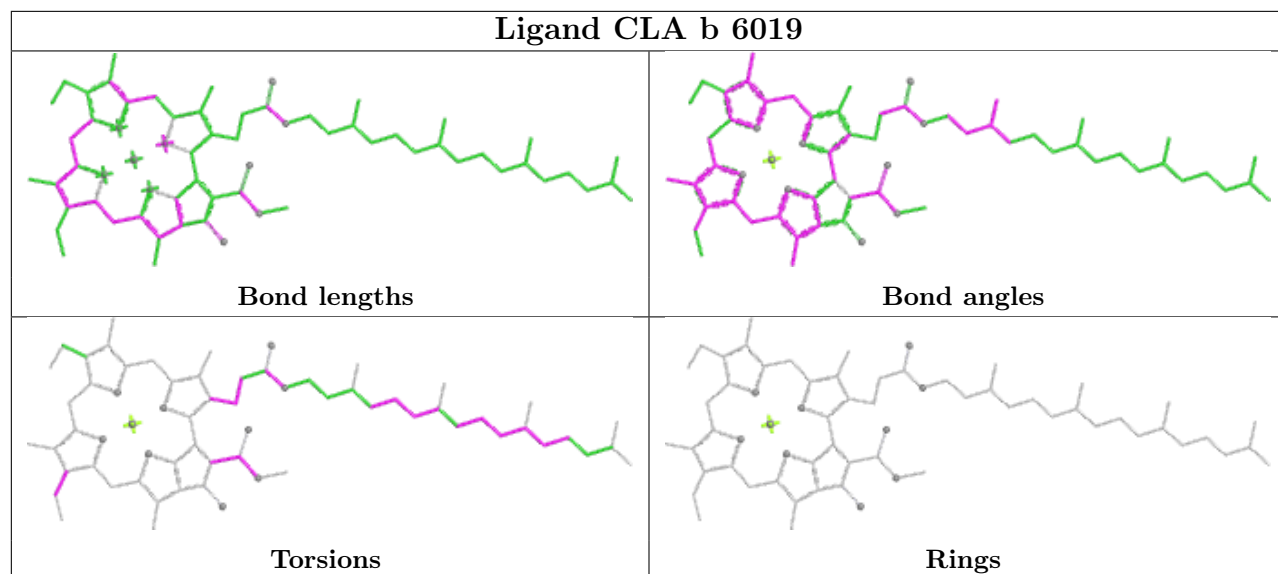


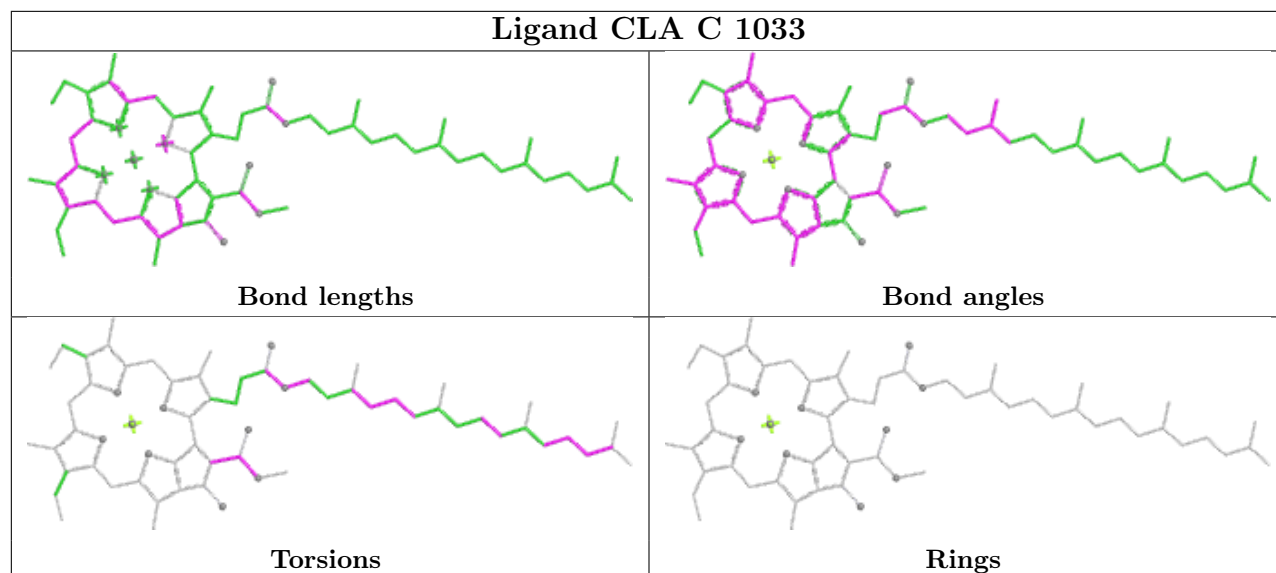
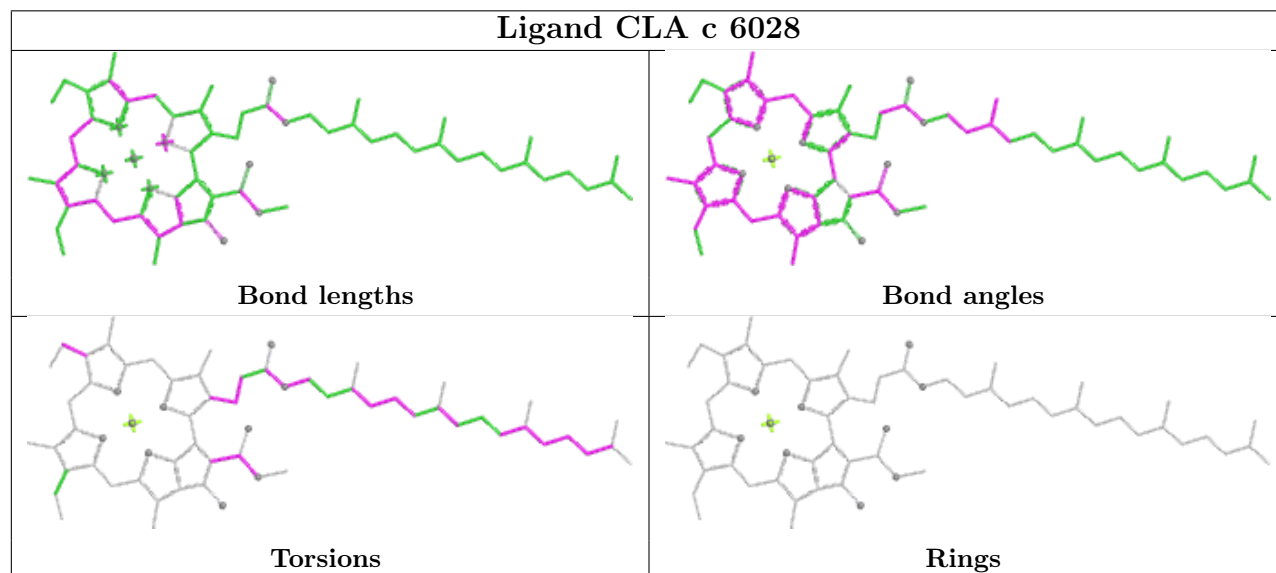
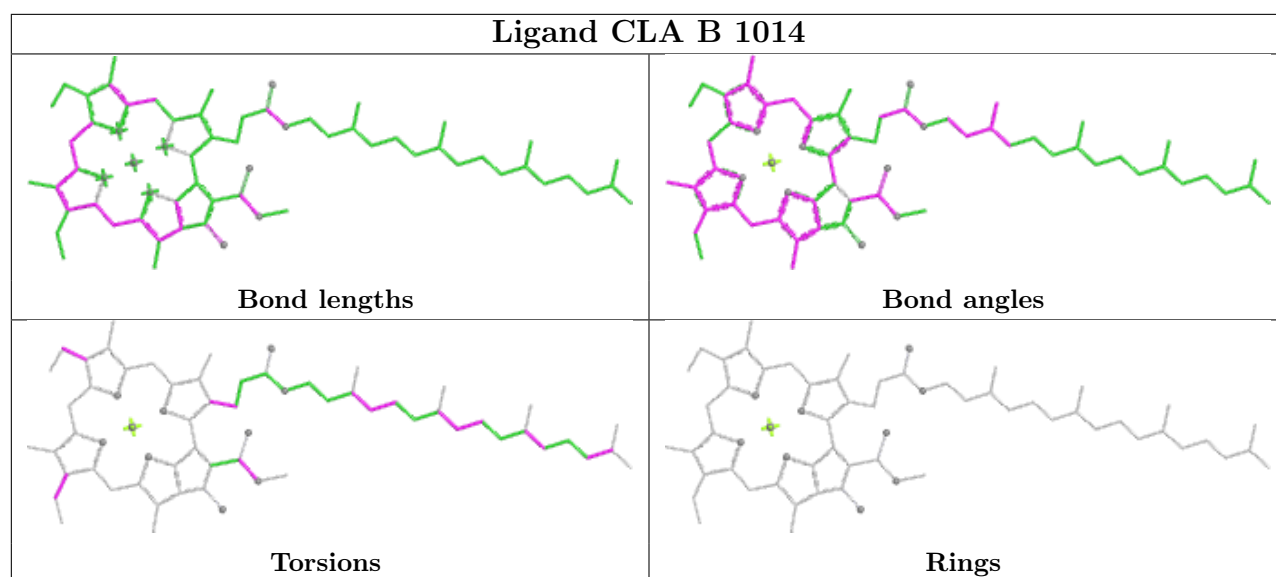
## Ligand CLA c 6030

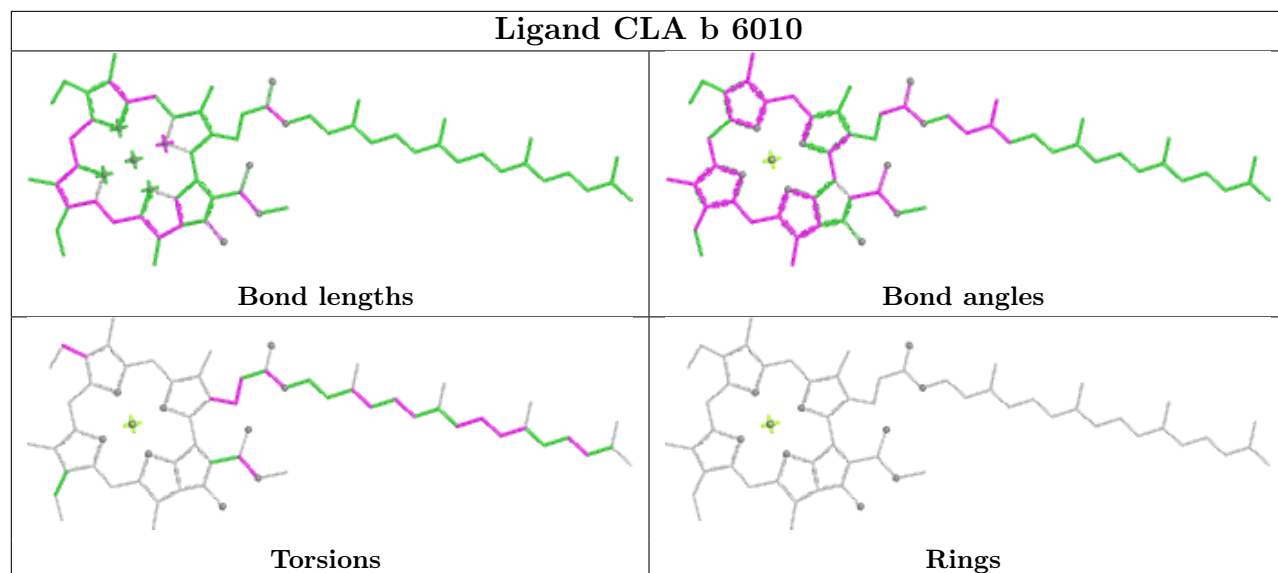
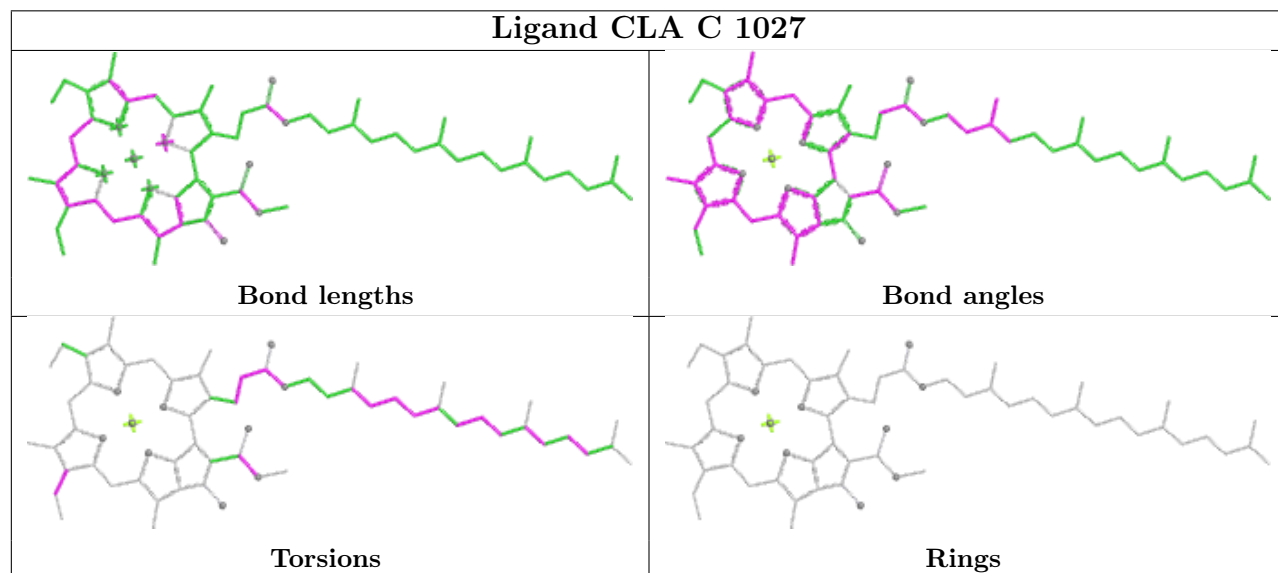
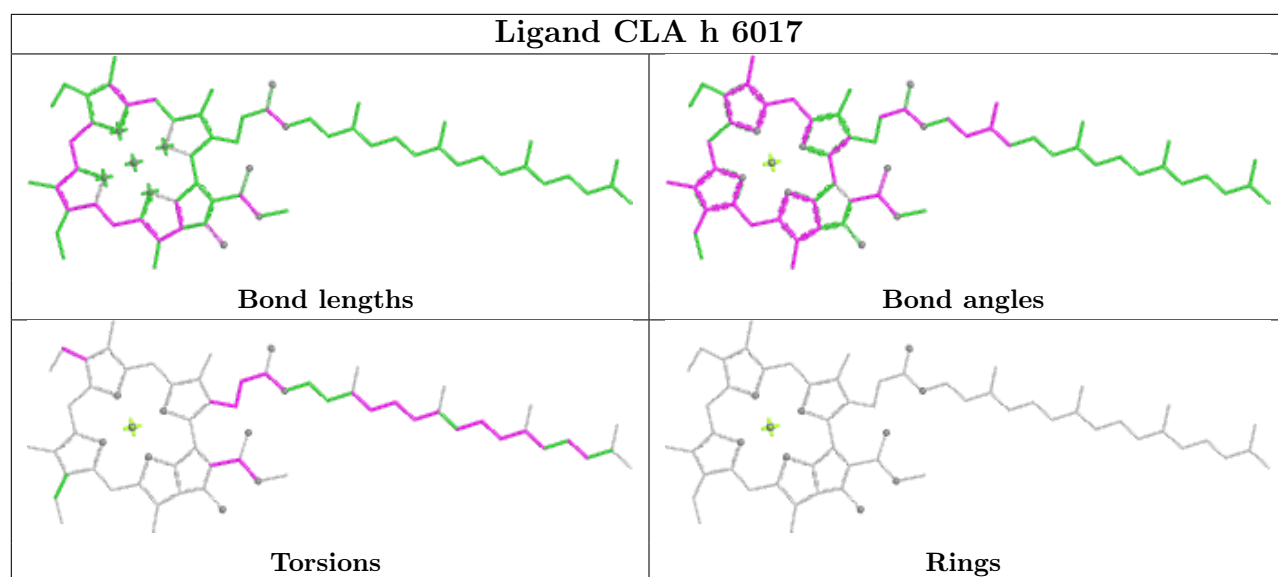


## Ligand CLA A 1003

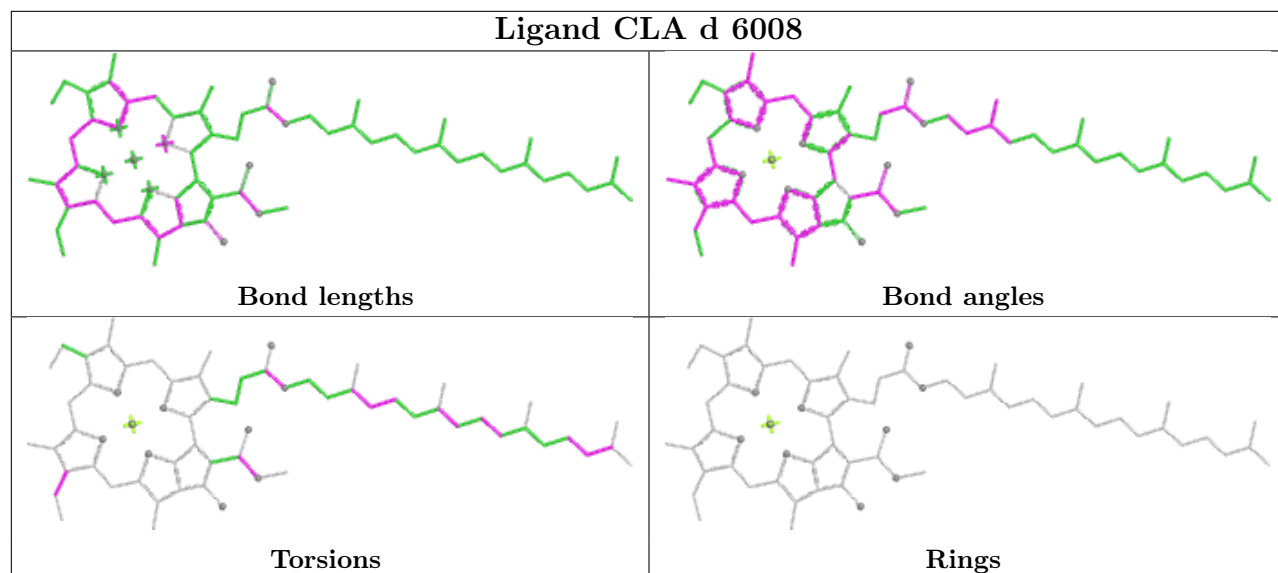
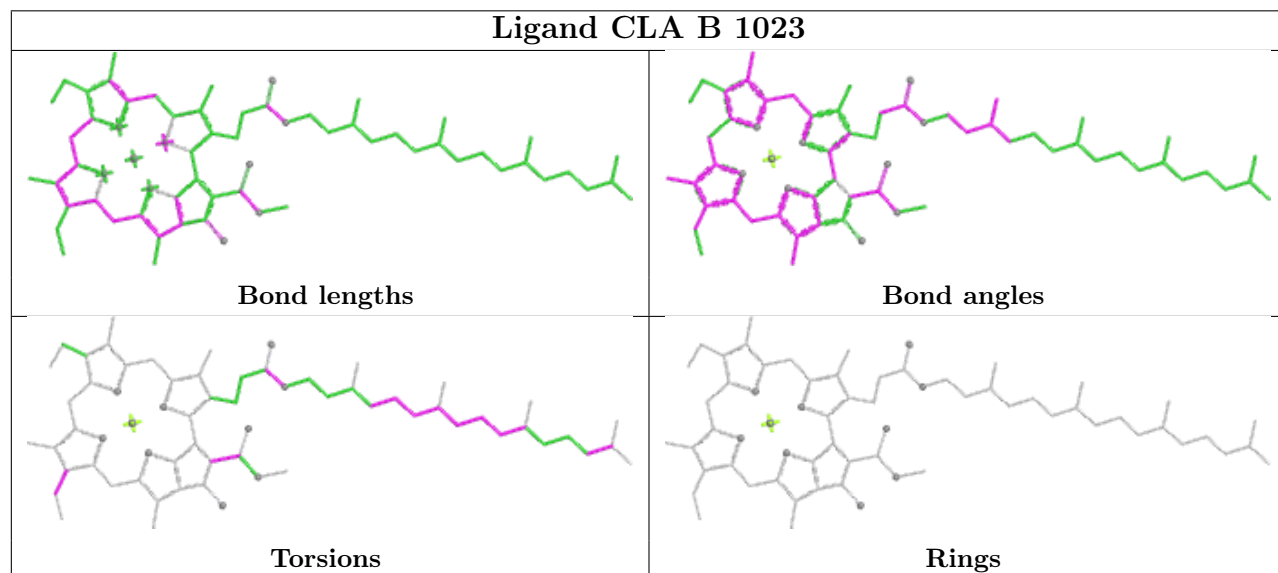
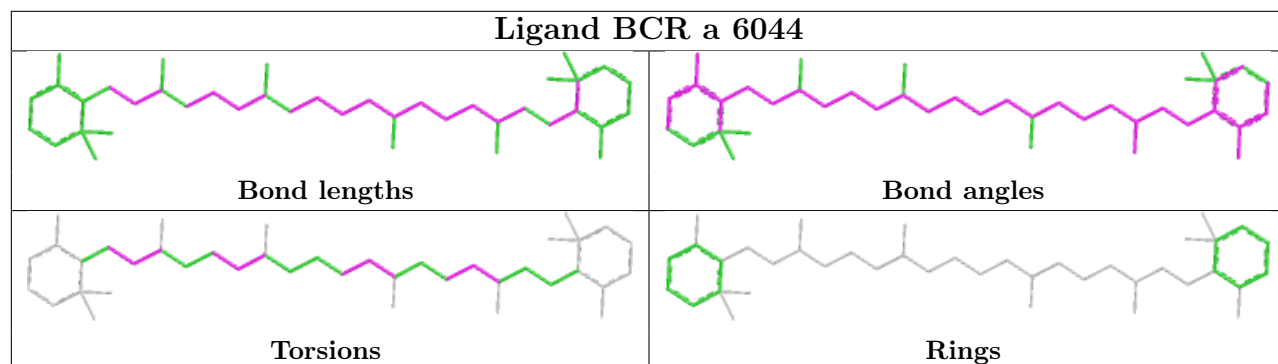


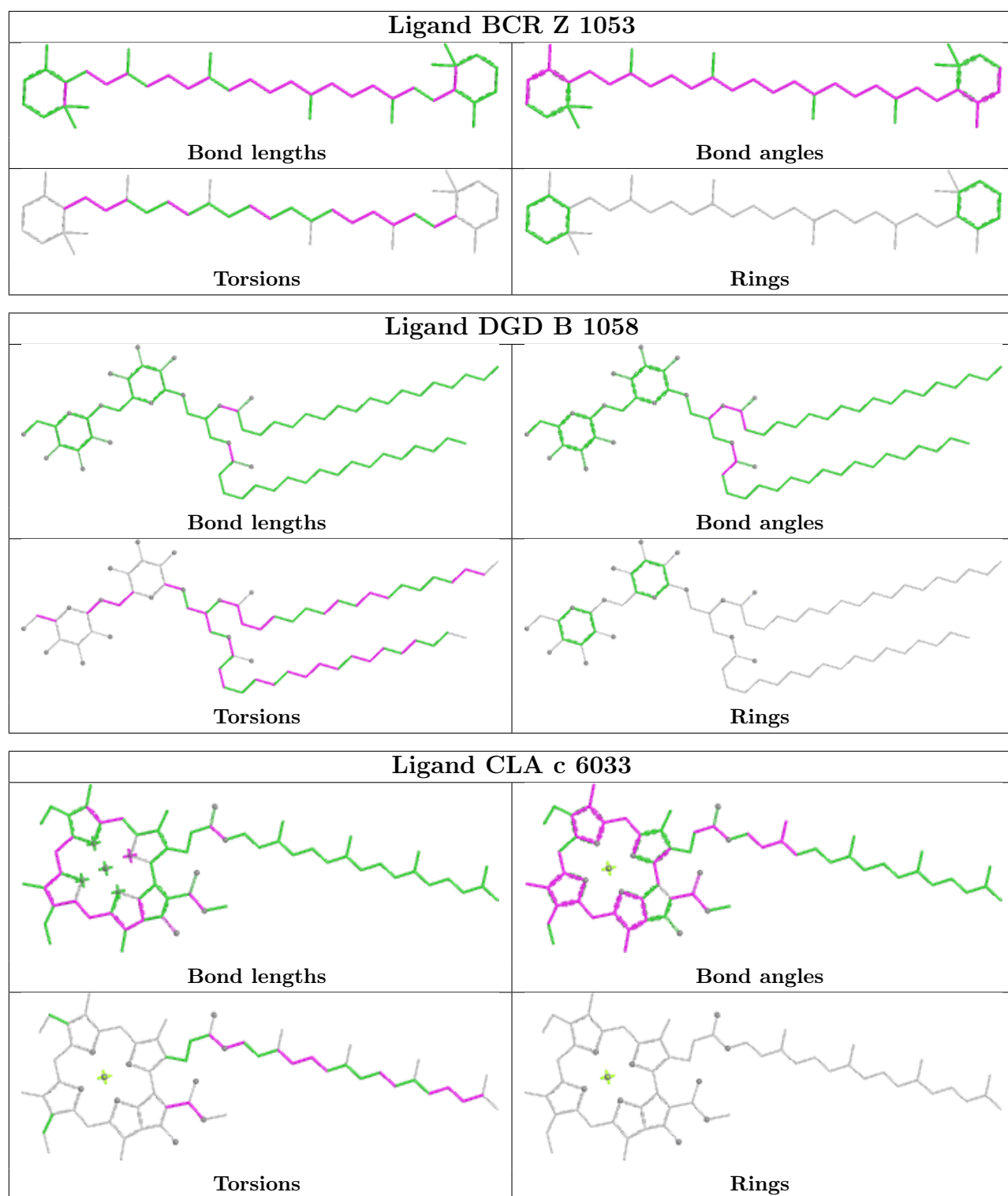


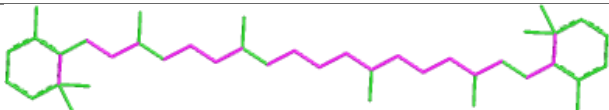
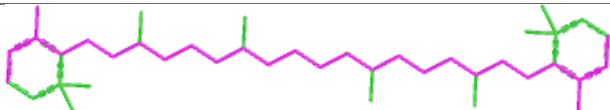
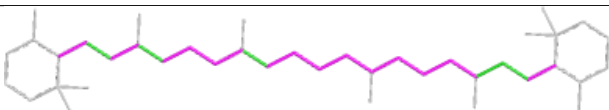
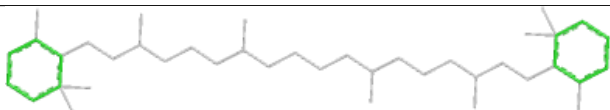


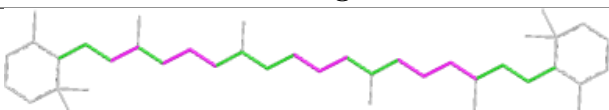
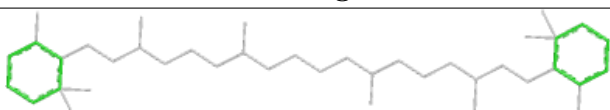


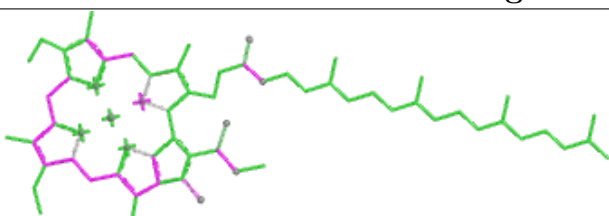
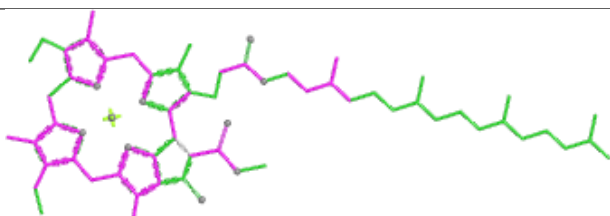
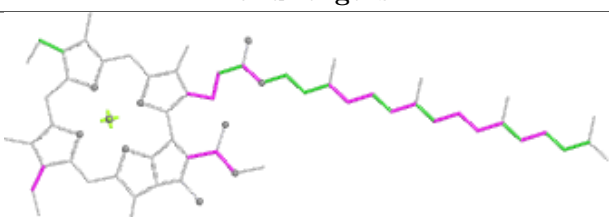
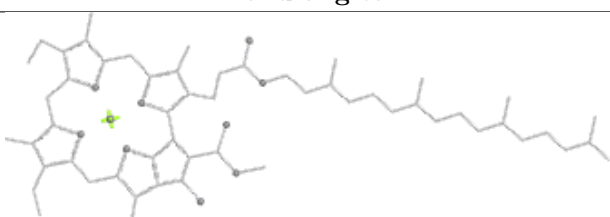




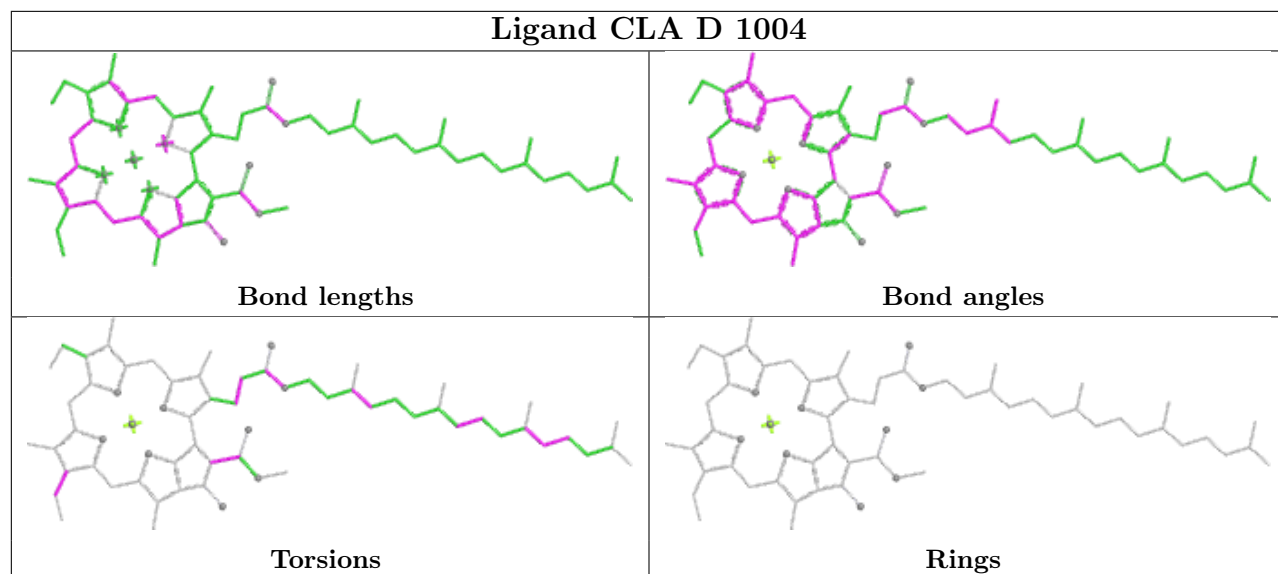


| Ligand BCR D 1050                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

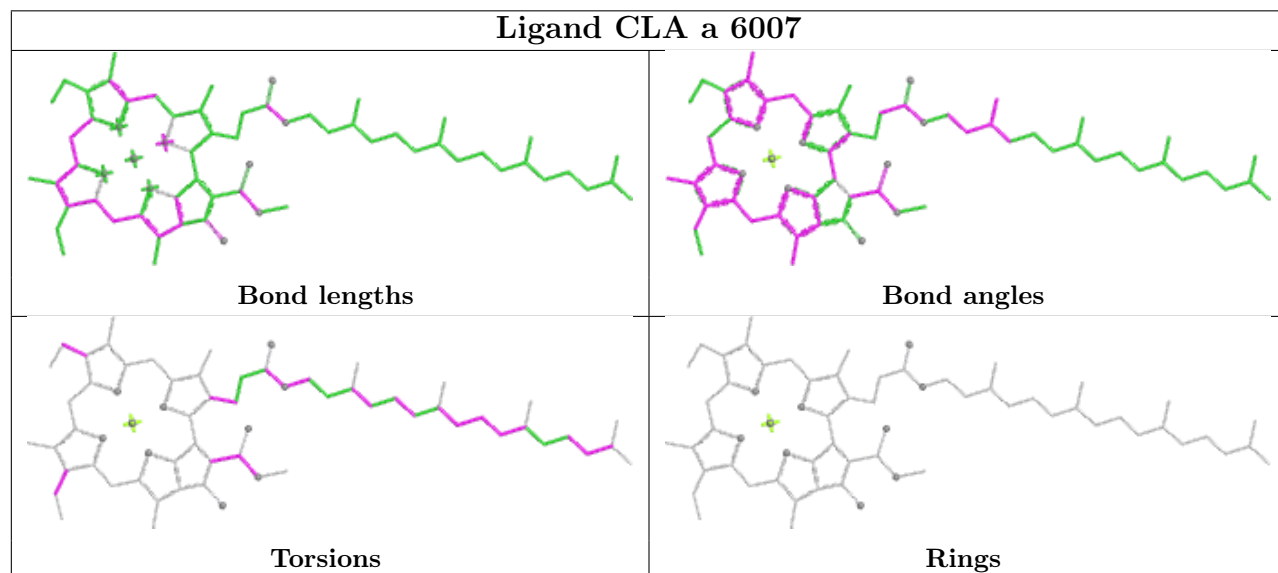
| Ligand BCR B 1048                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA c 6032                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

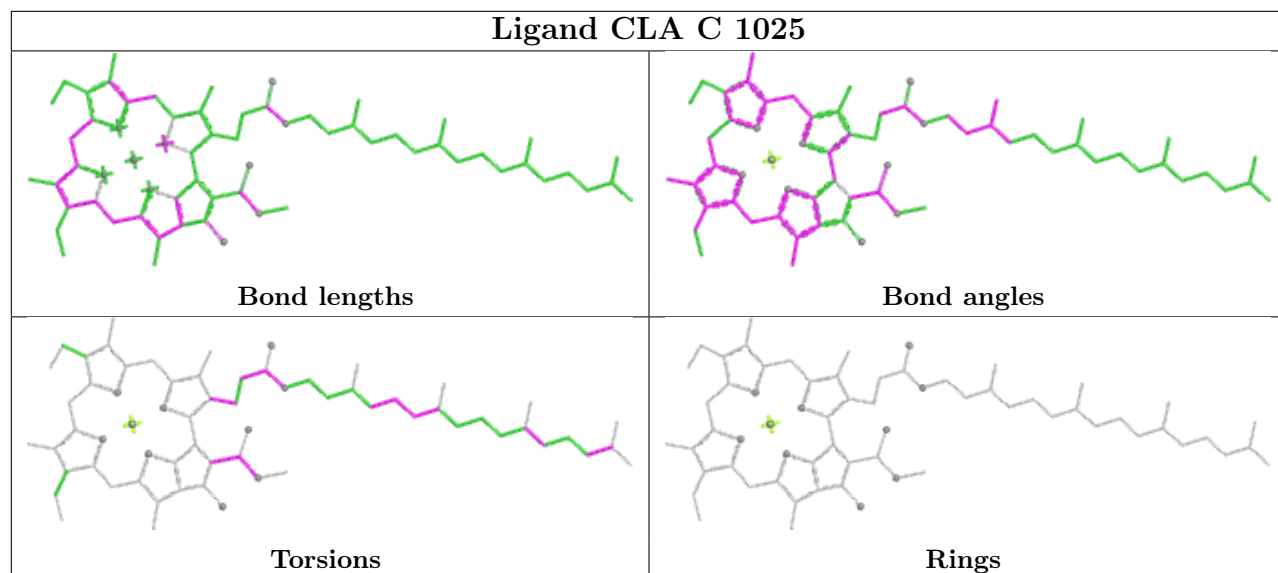
## Ligand CLA D 1004



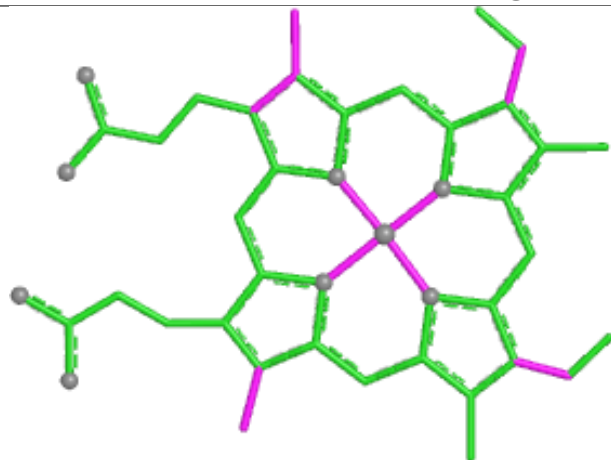
## Ligand CLA a 6007



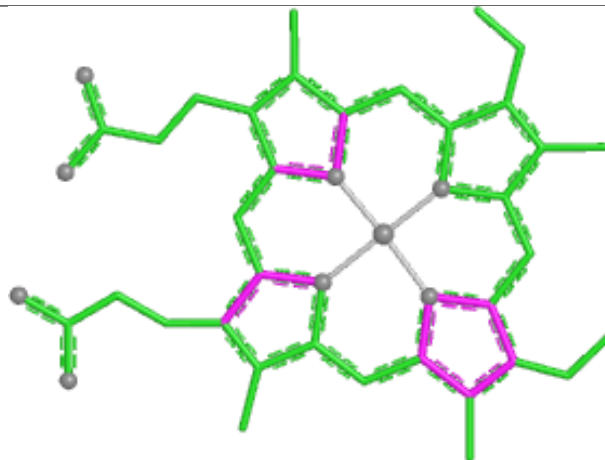
## Ligand CLA C 1025



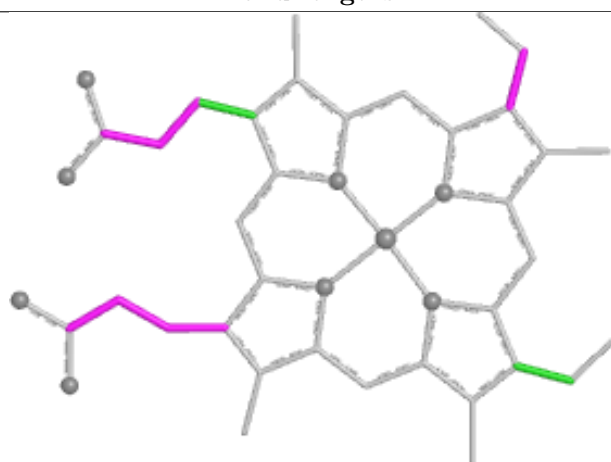
## Ligand HEM f 6040



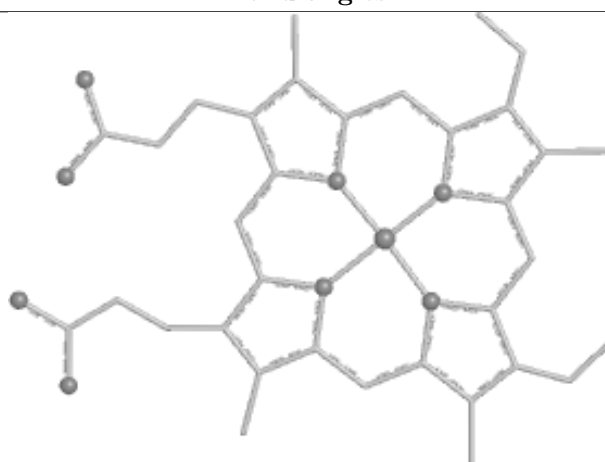
Bond lengths



Bond angles

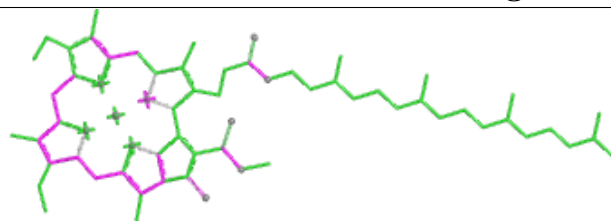


Torsions

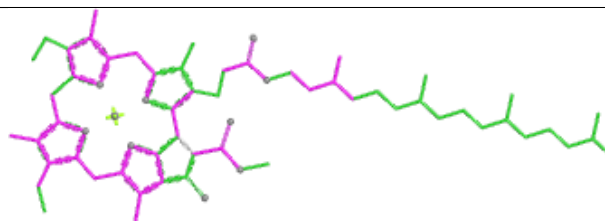


Rings

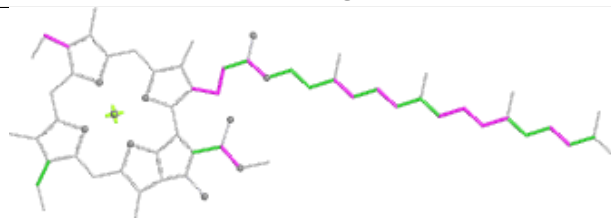
## Ligand CLA B 1010



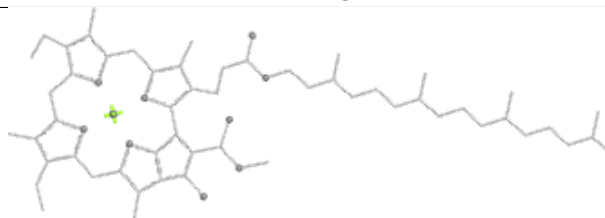
Bond lengths



Bond angles

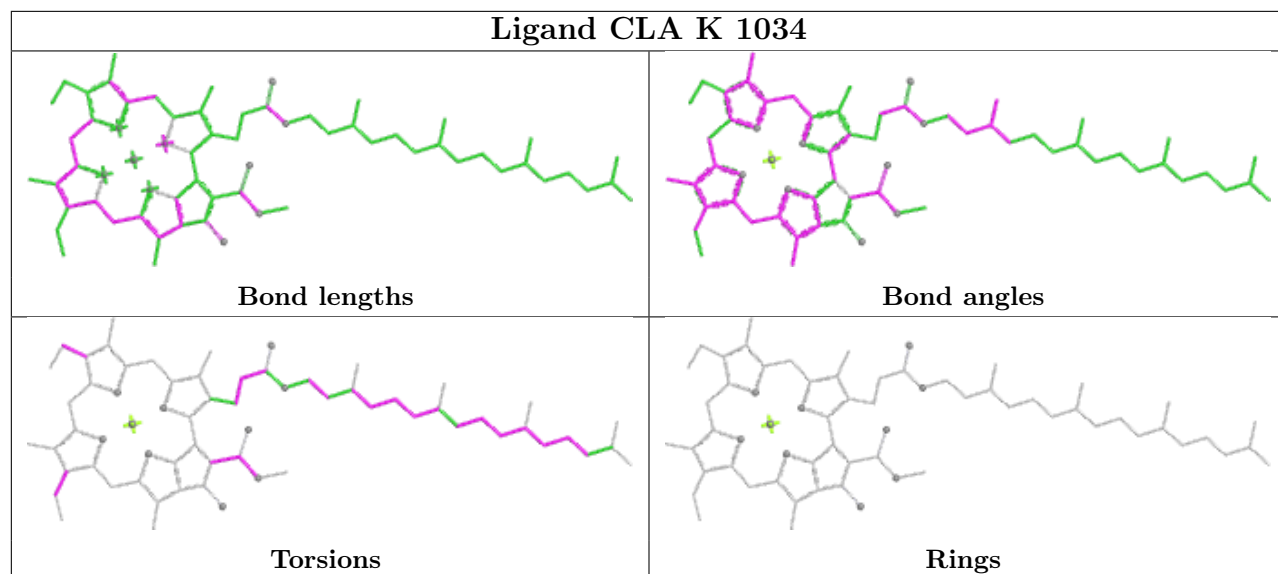


Torsions

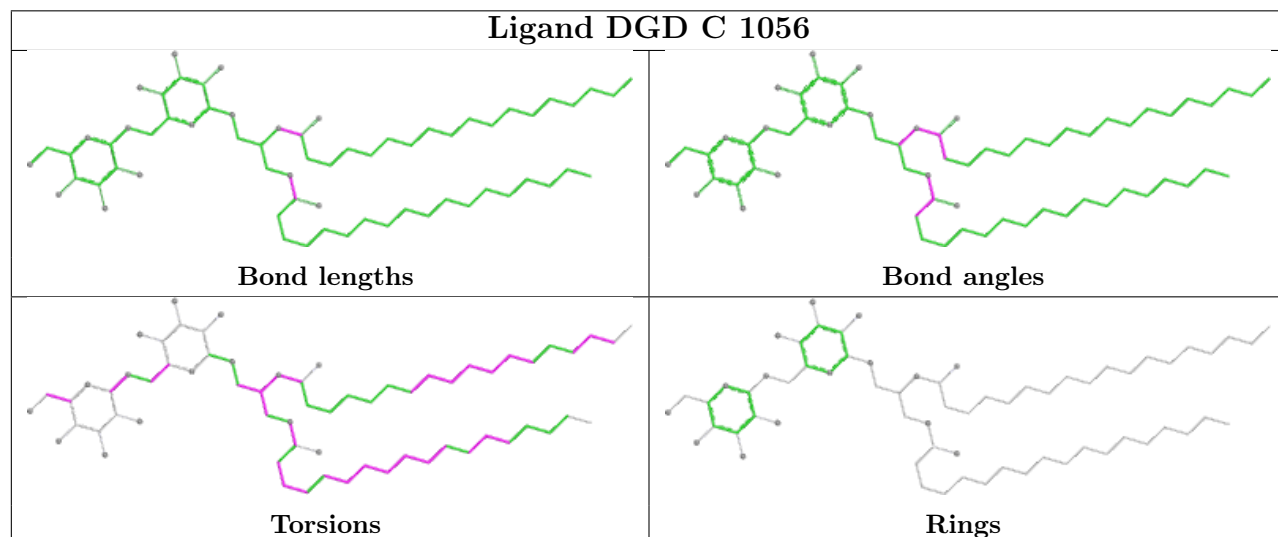


Rings

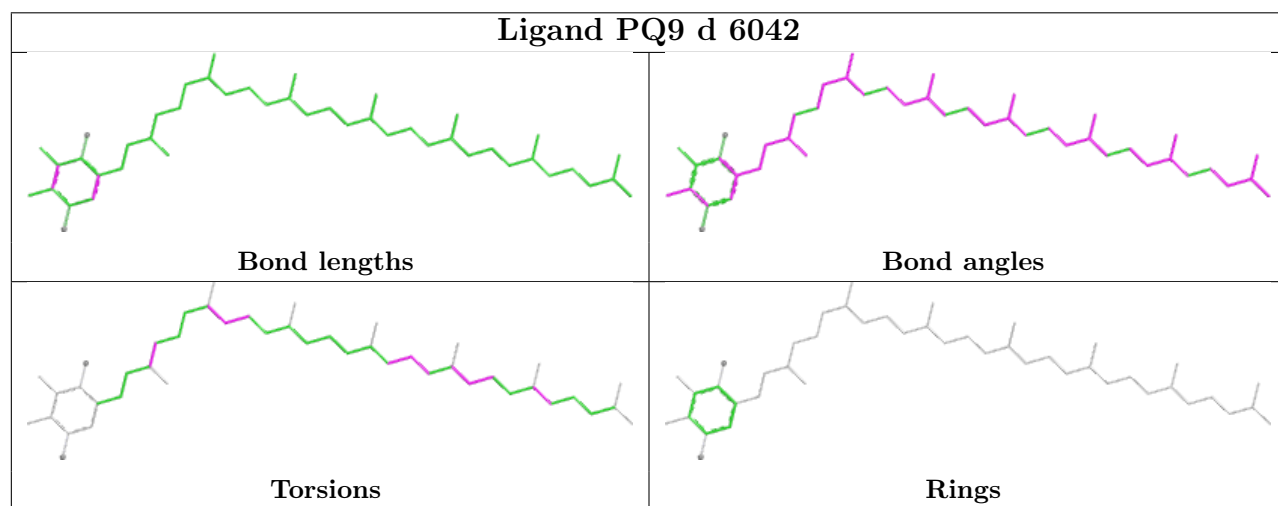
## Ligand CLA K 1034

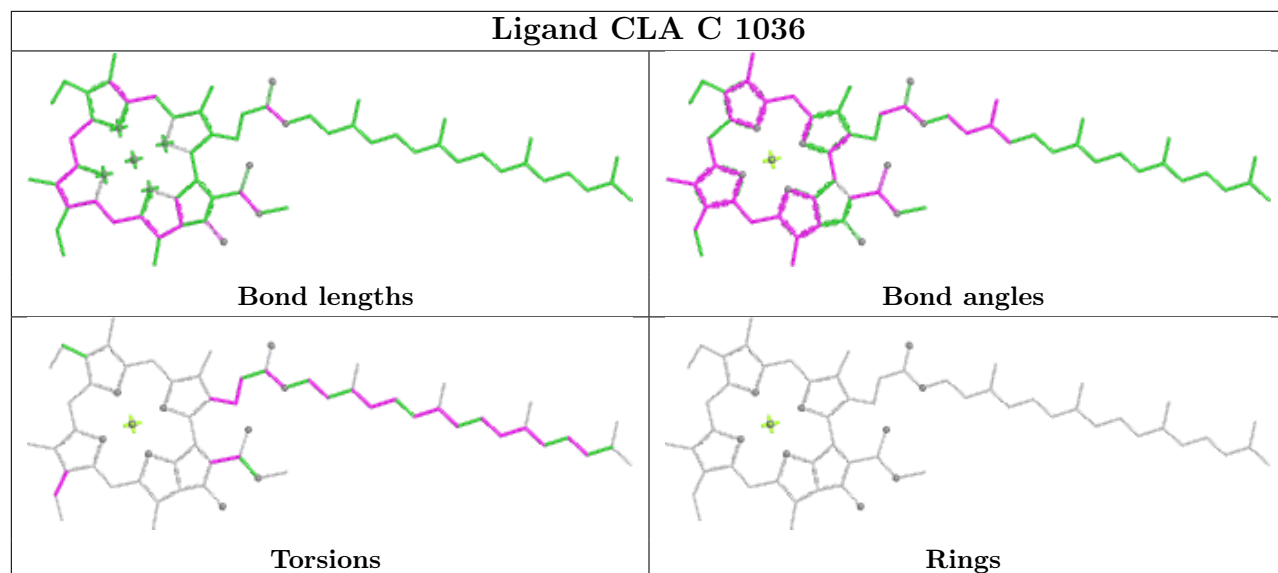
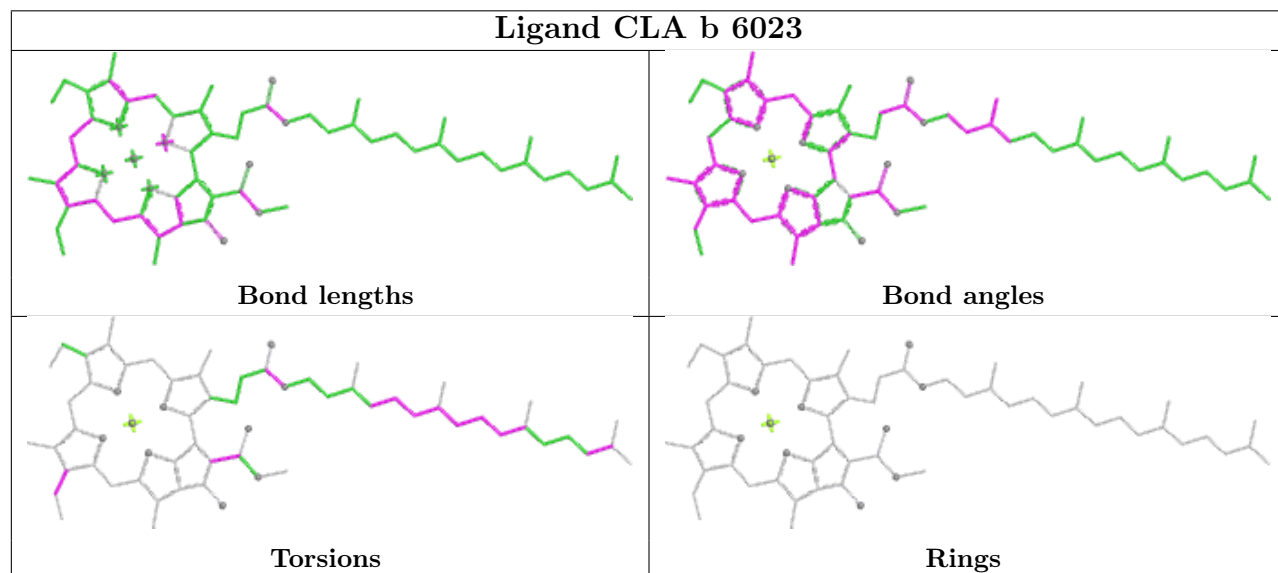
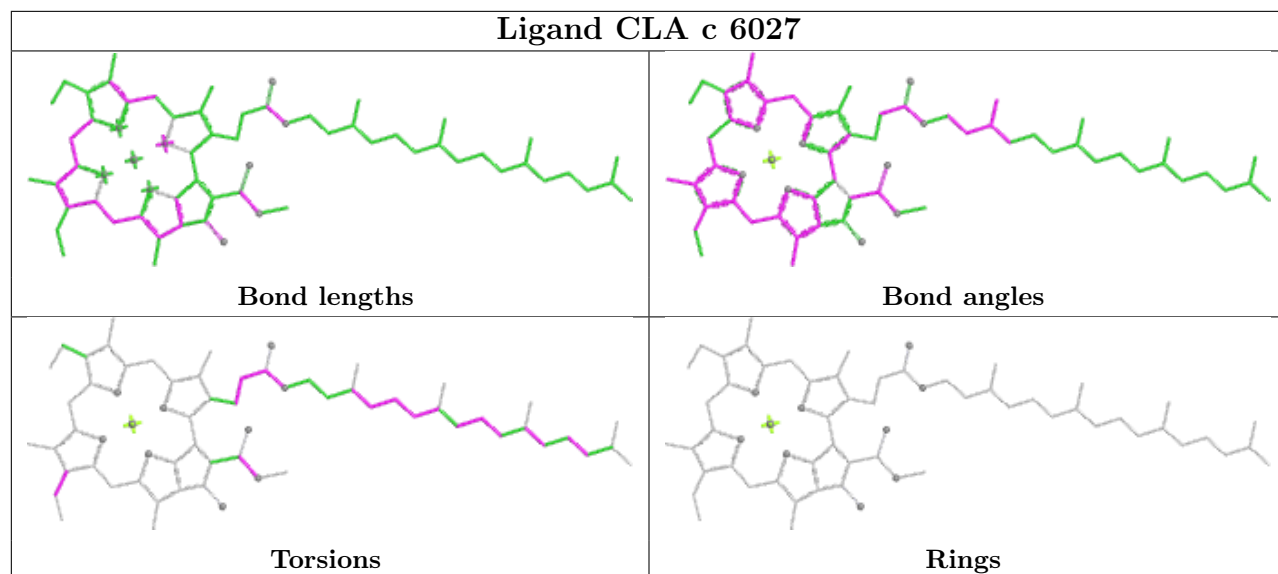


## Ligand DGD C 1056



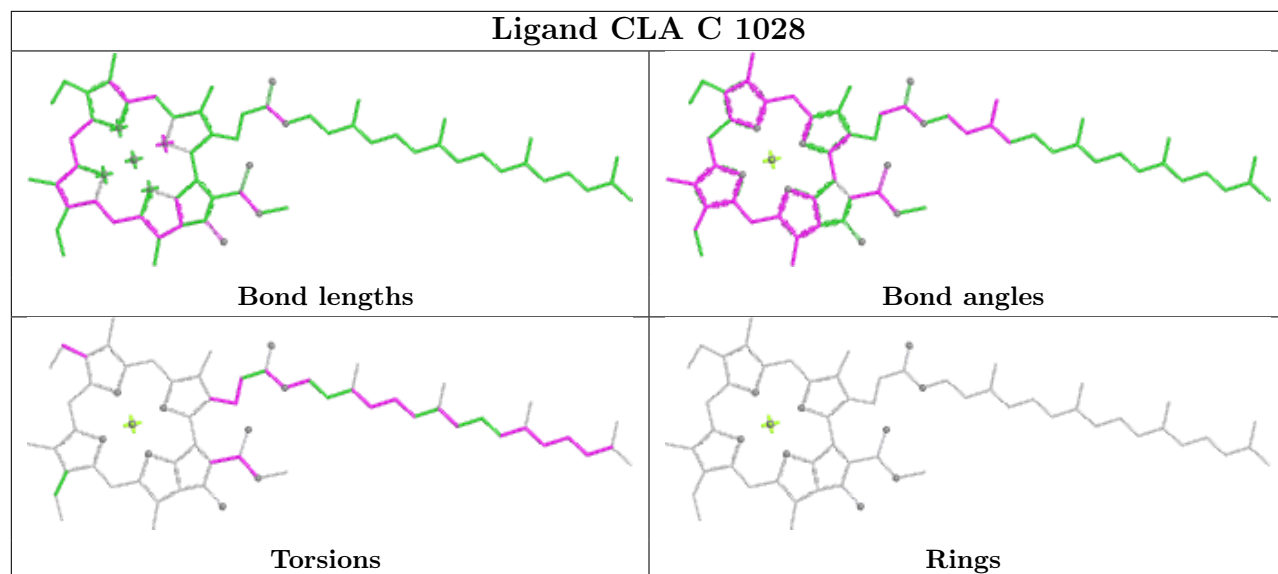
## Ligand PQ9 d 6042



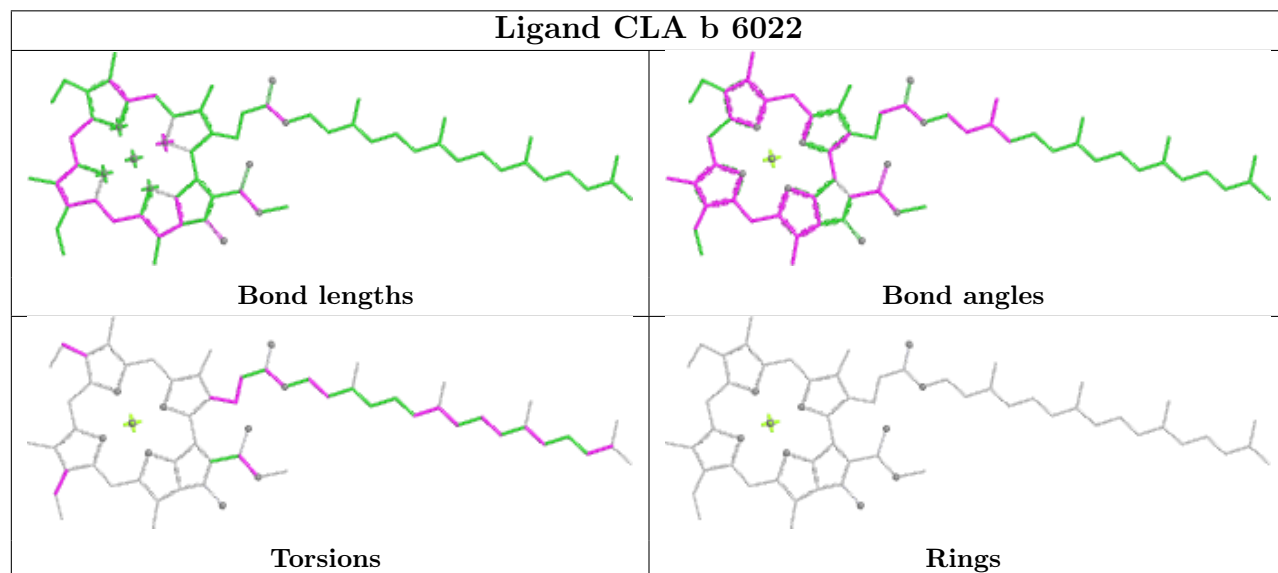




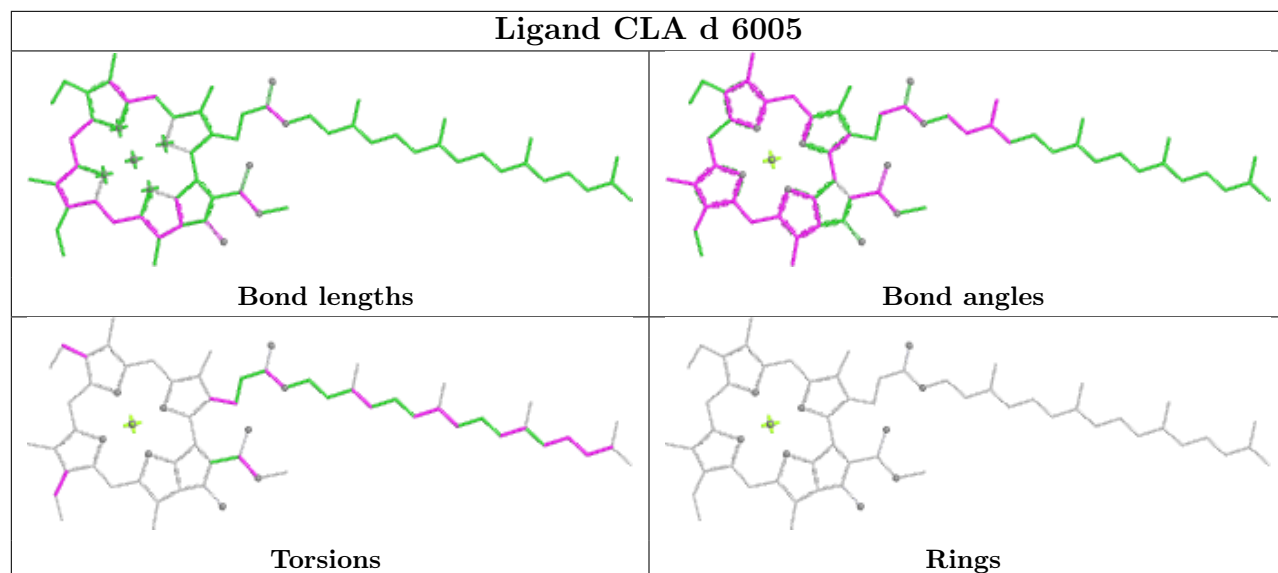
## Ligand CLA C 1028

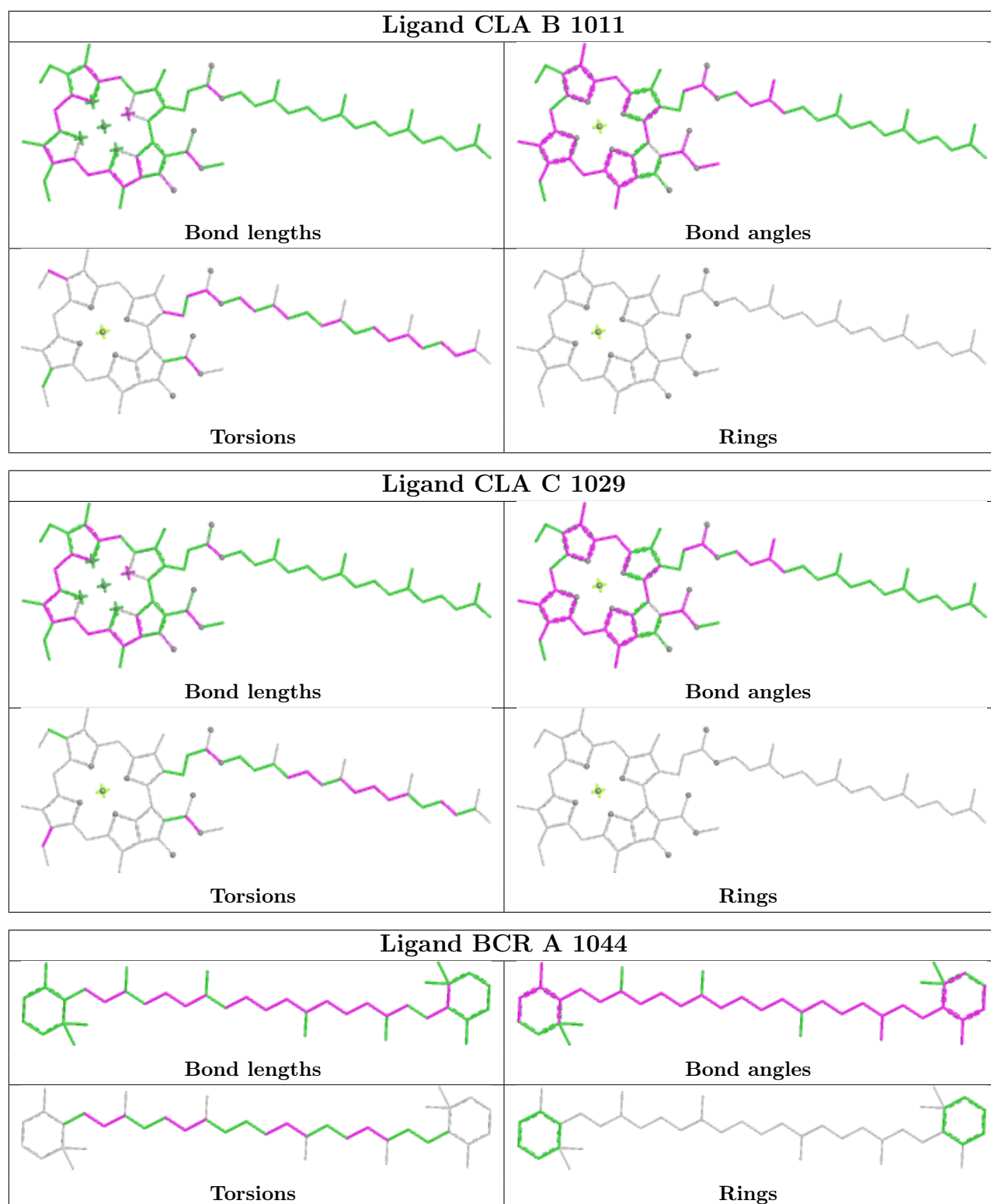


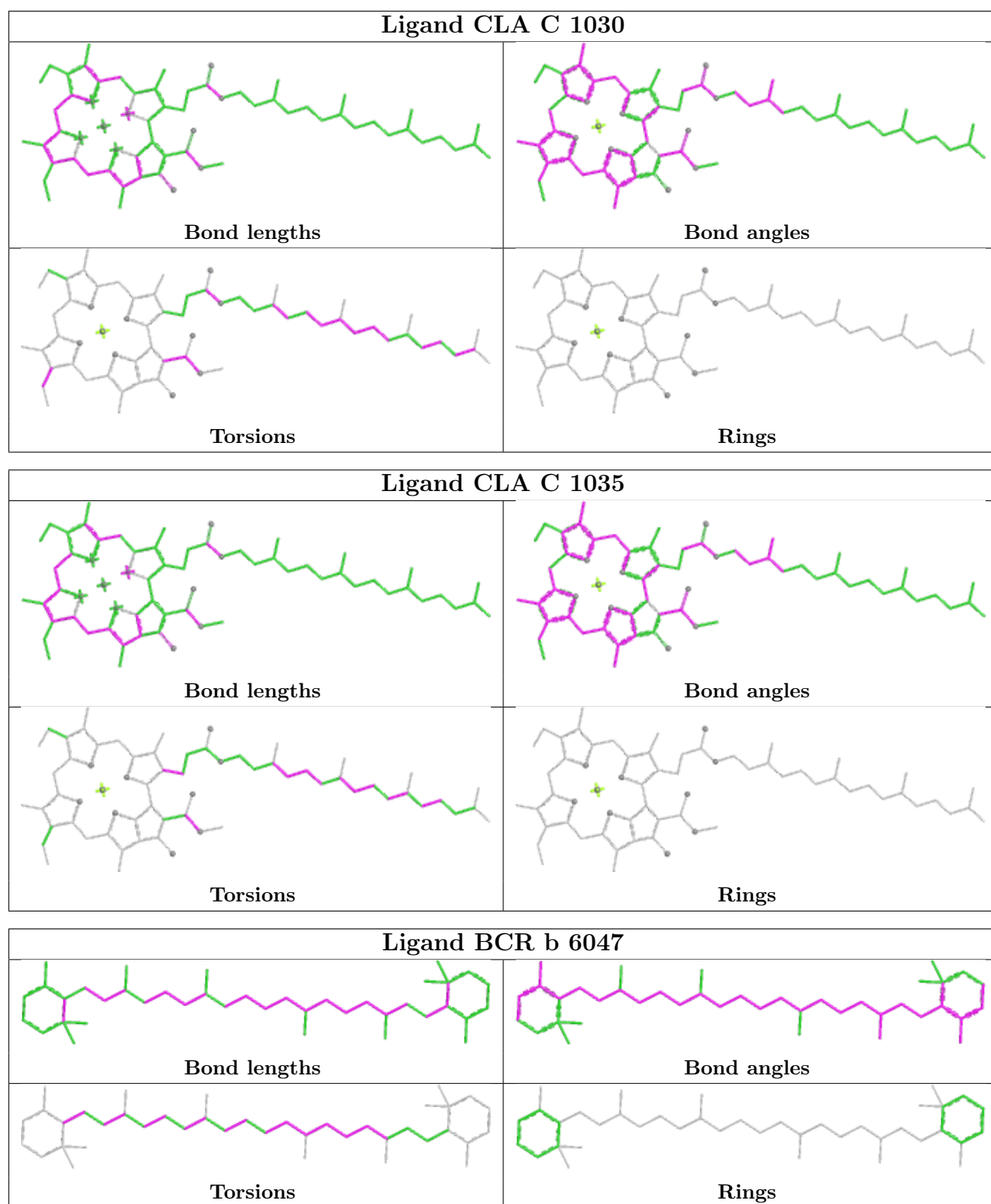
## Ligand CLA b 6022

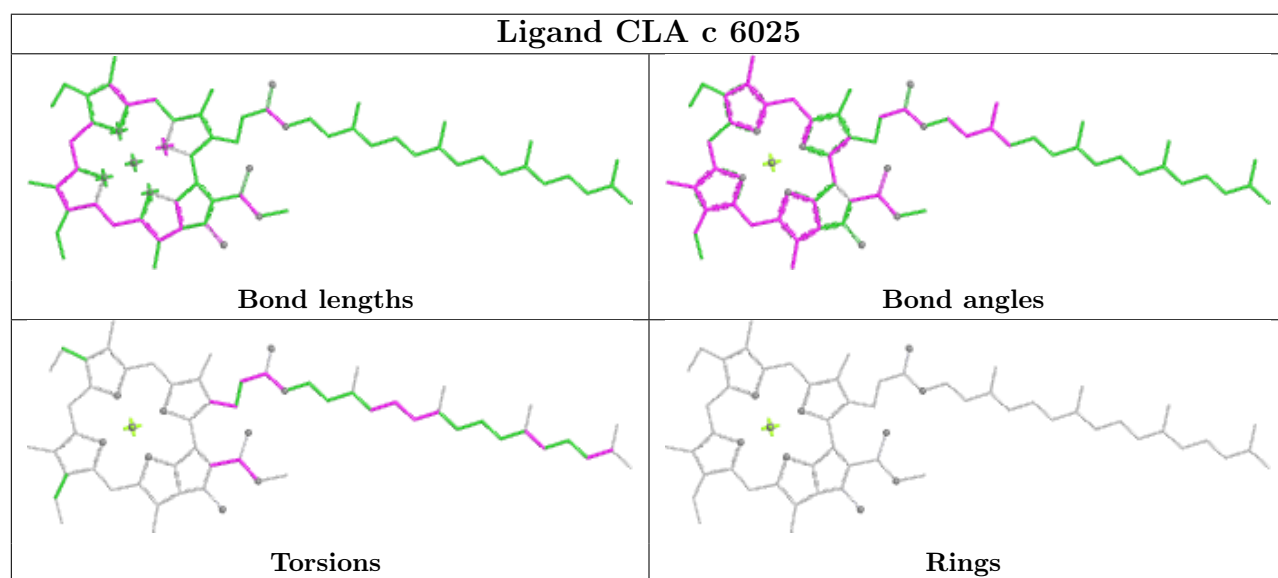
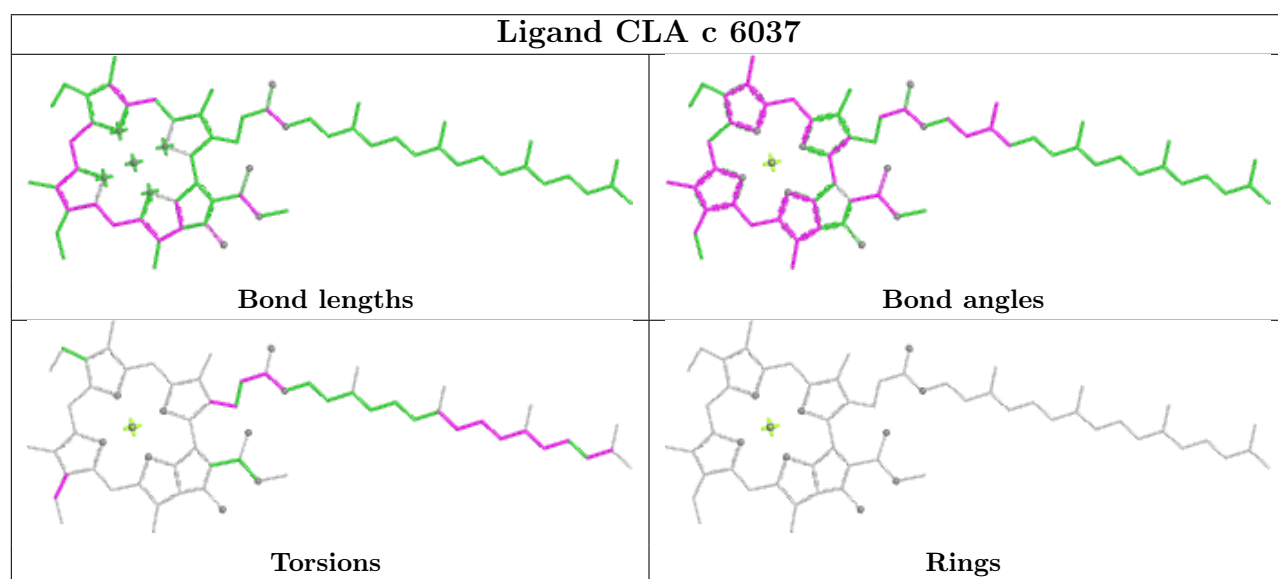
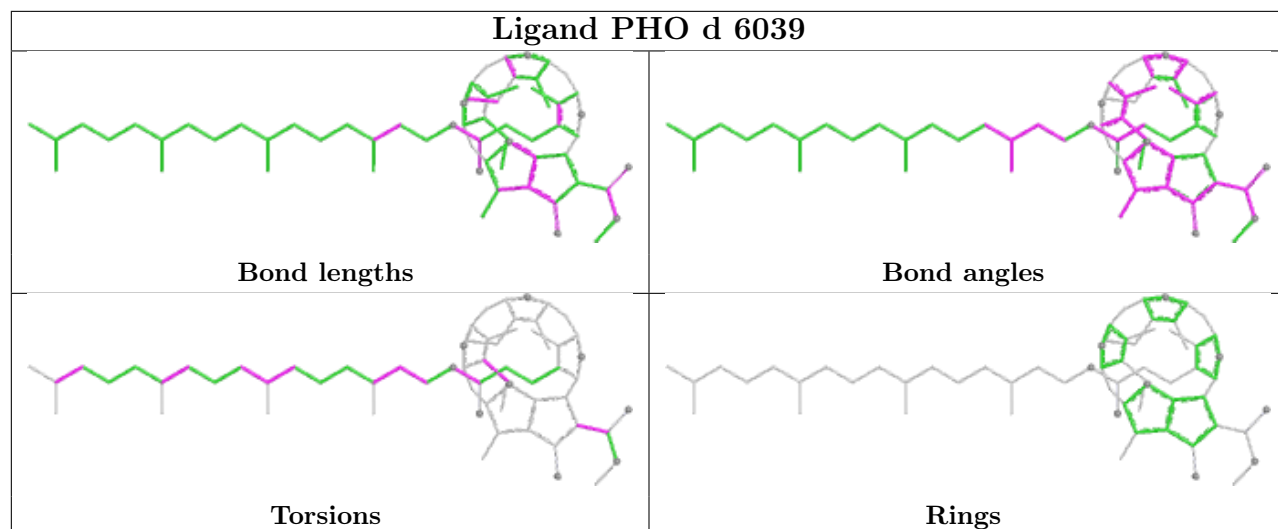


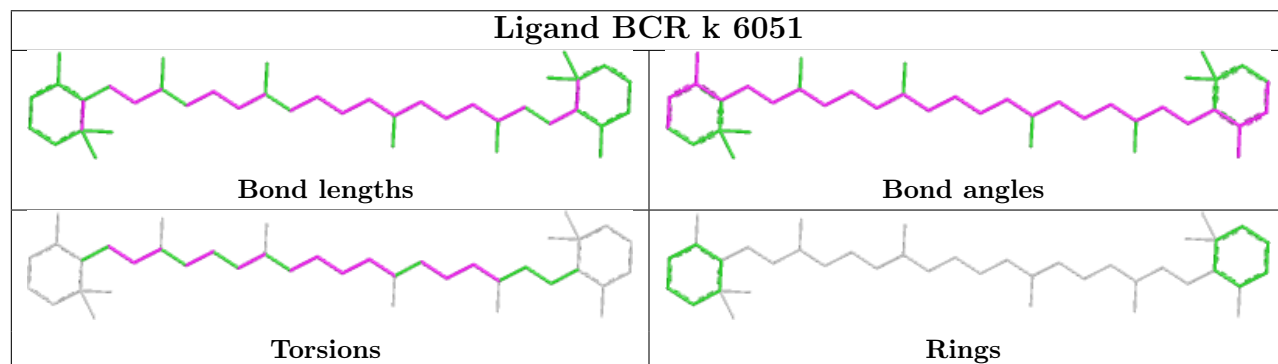
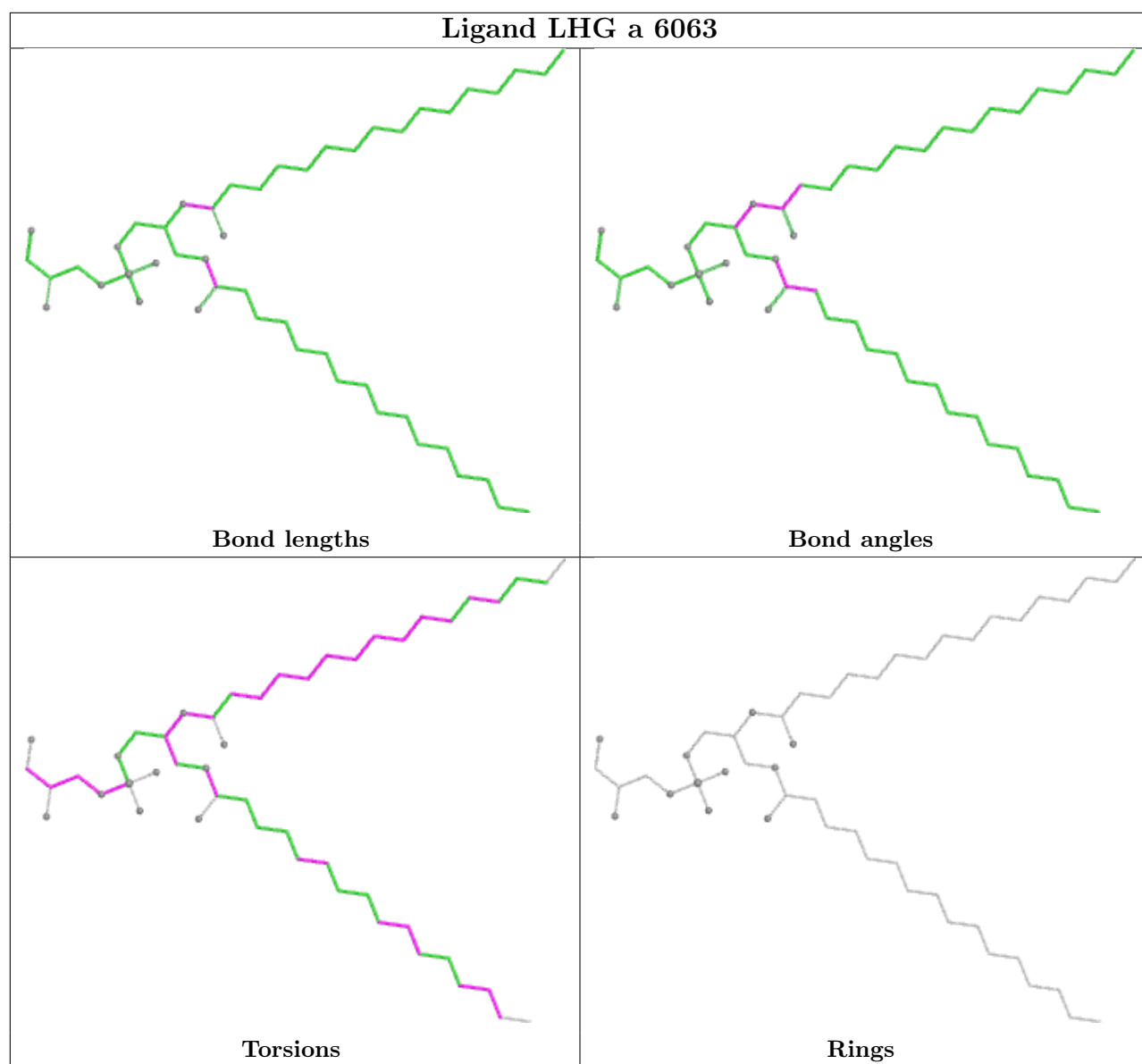
## Ligand CLA d 6005



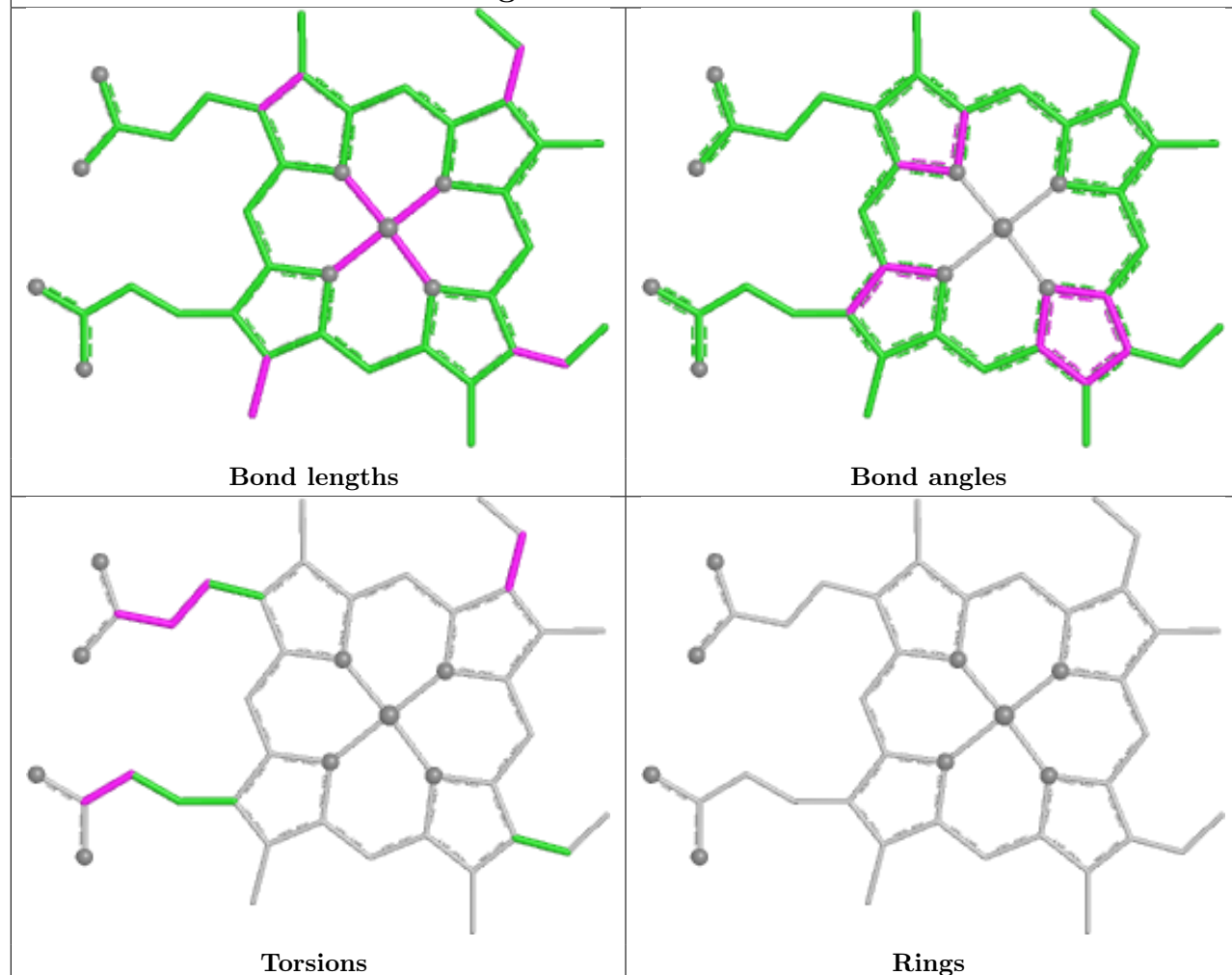




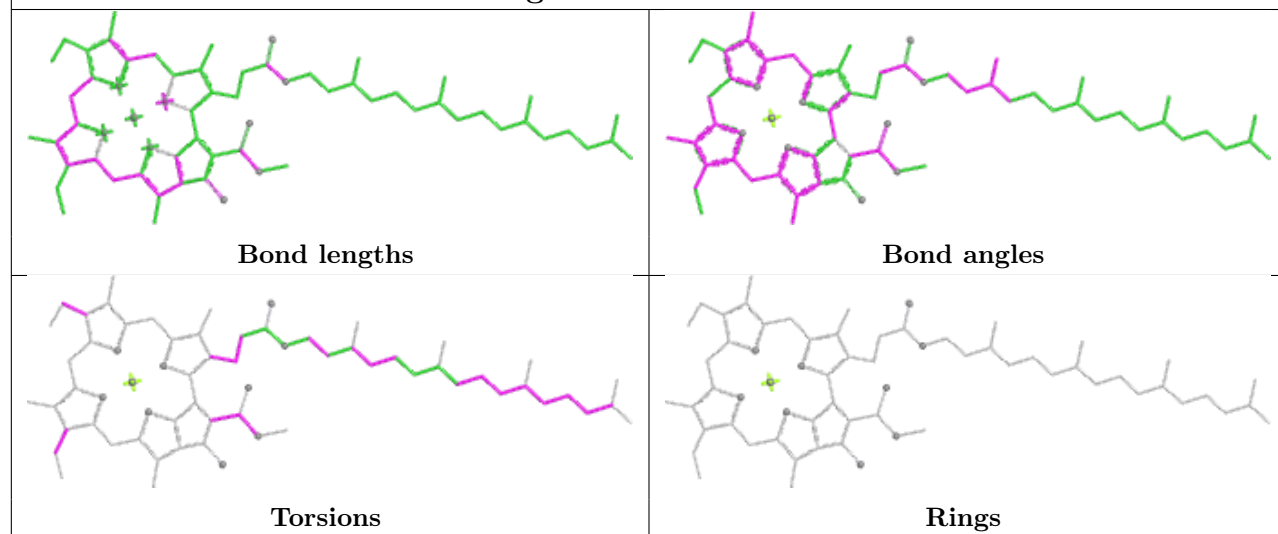




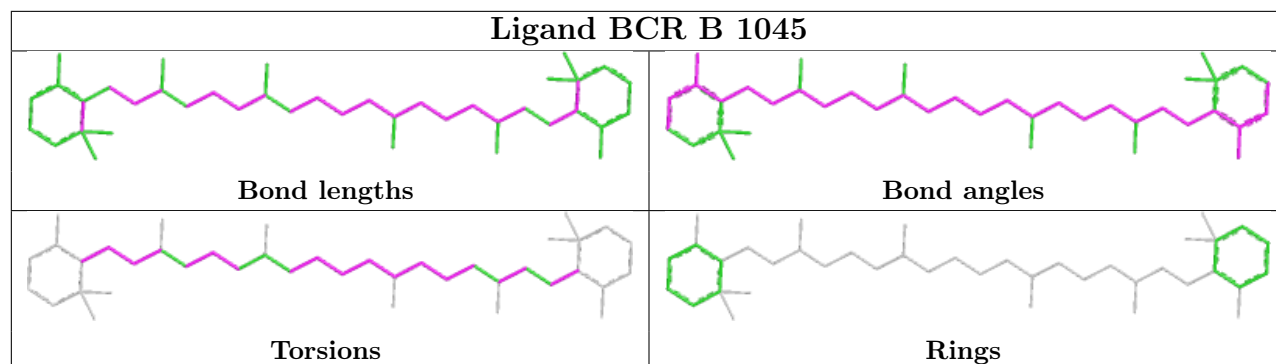
## Ligand HEM V 1041



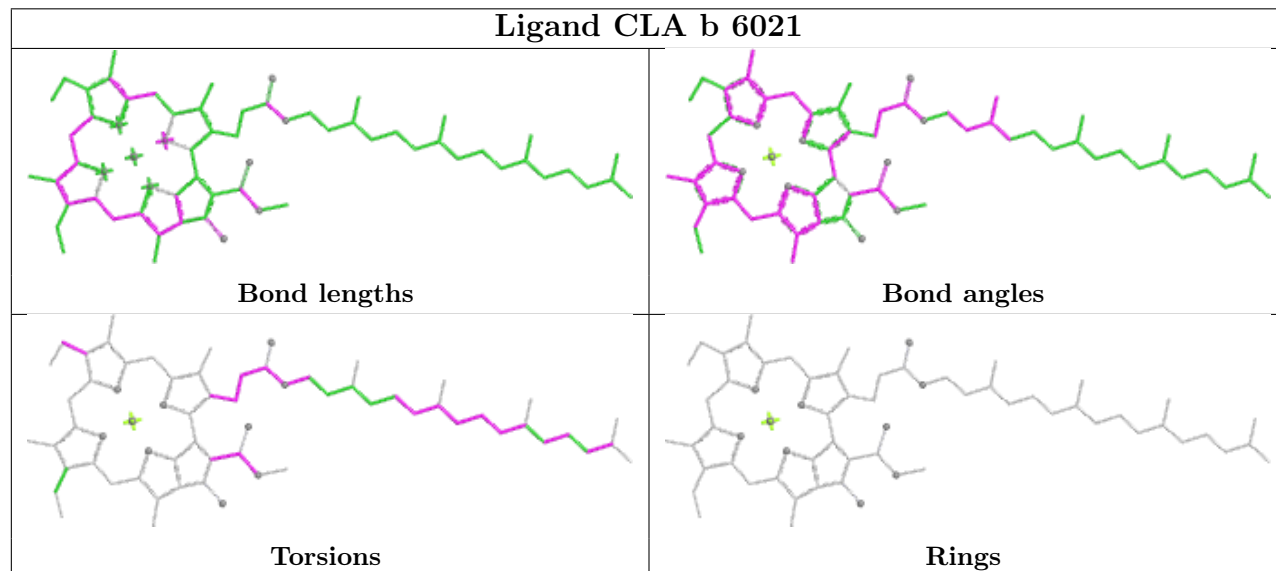
## Ligand CLA b 6013



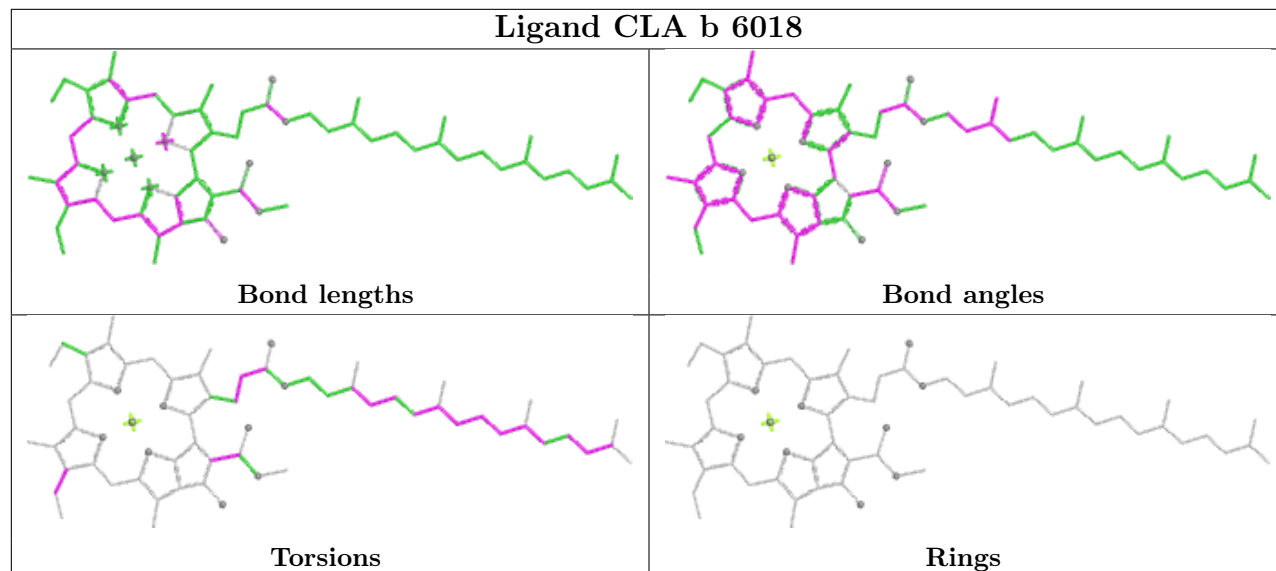
## Ligand BCR B 1045



## Ligand CLA b 6021

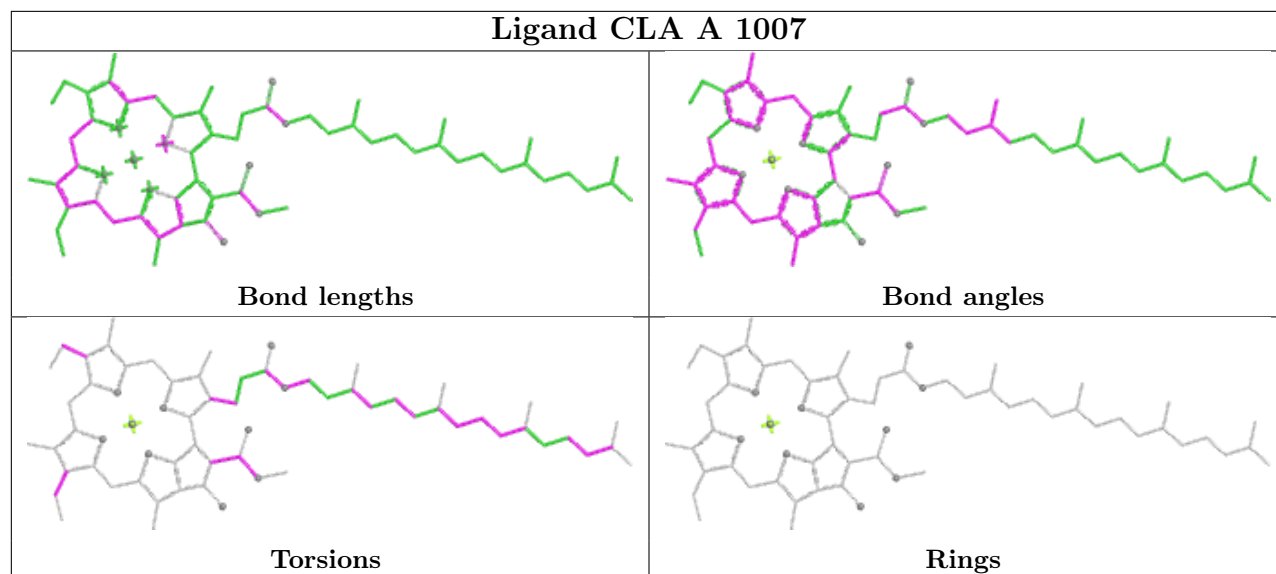


## Ligand CLA b 6018

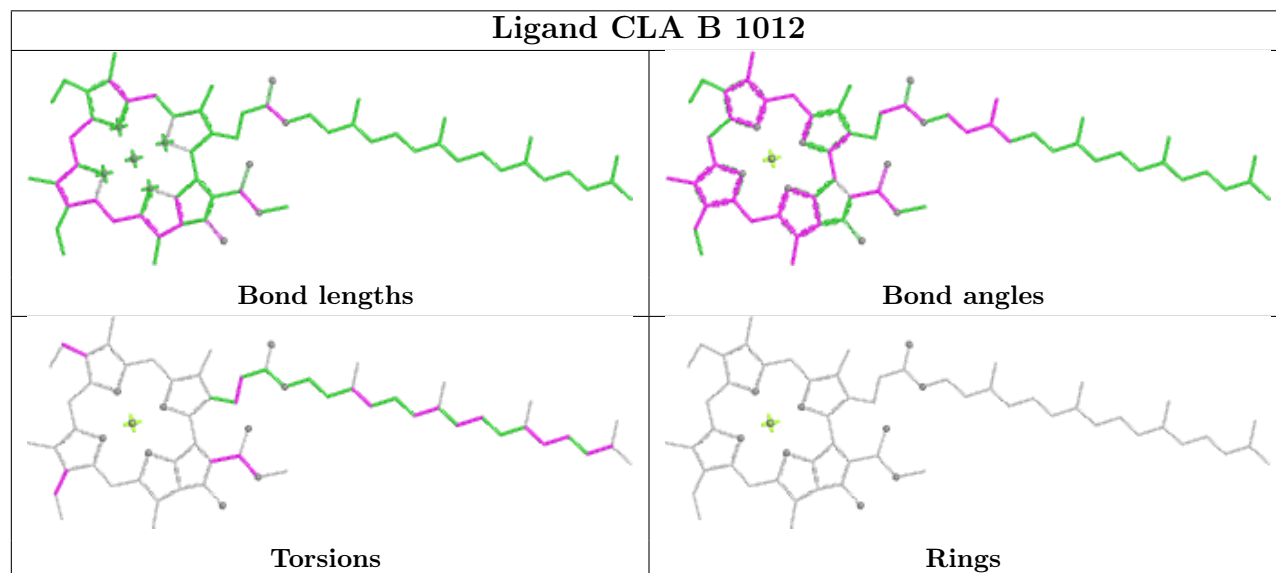




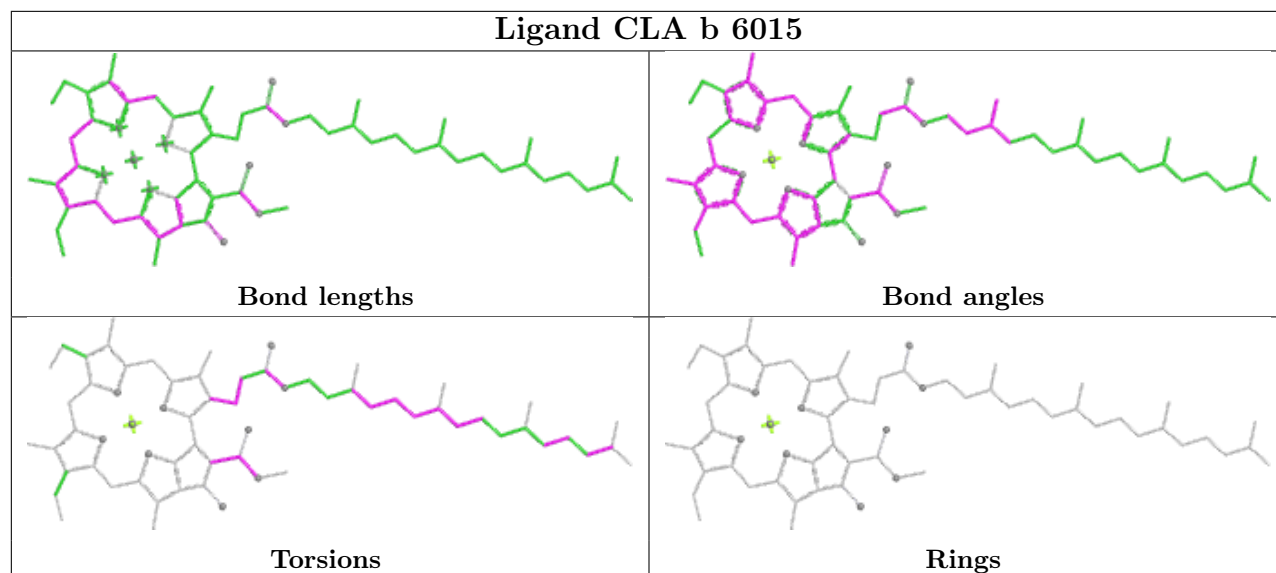
## Ligand CLA A 1007



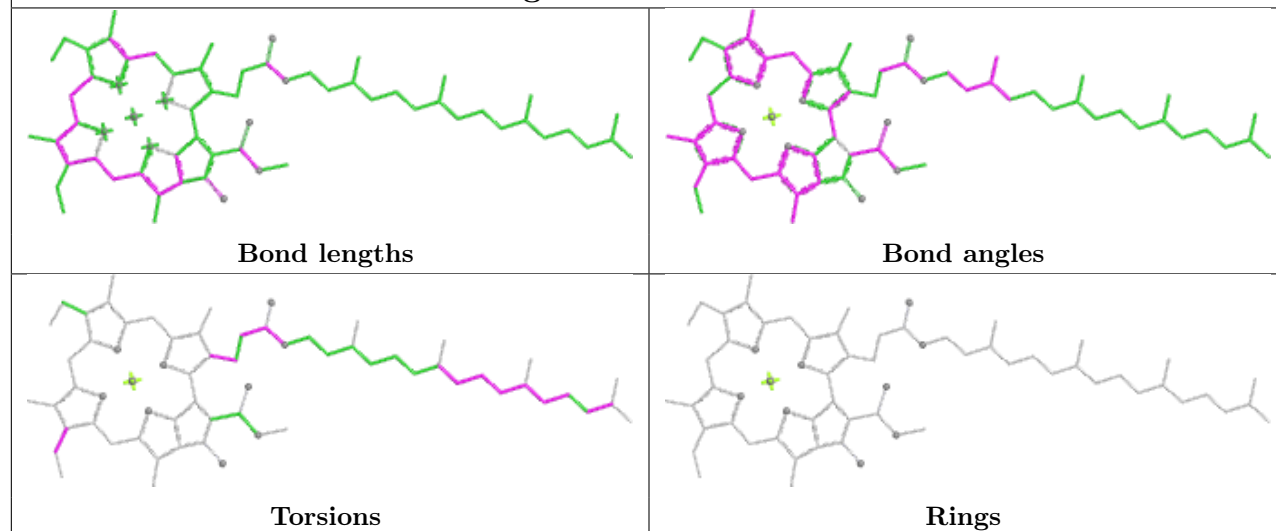
## Ligand CLA B 1012



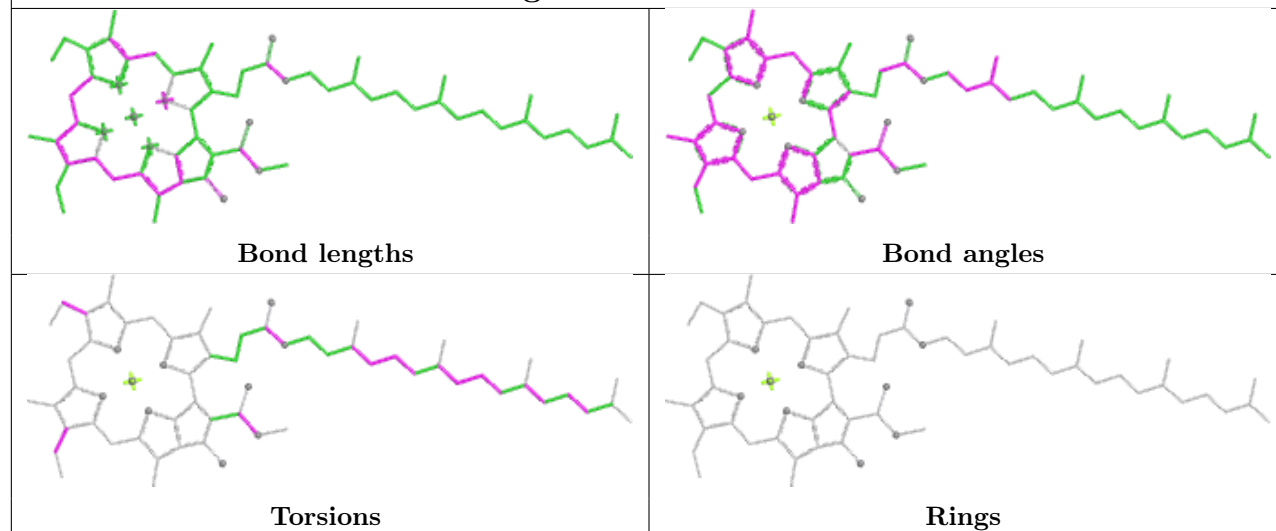
## Ligand CLA b 6015



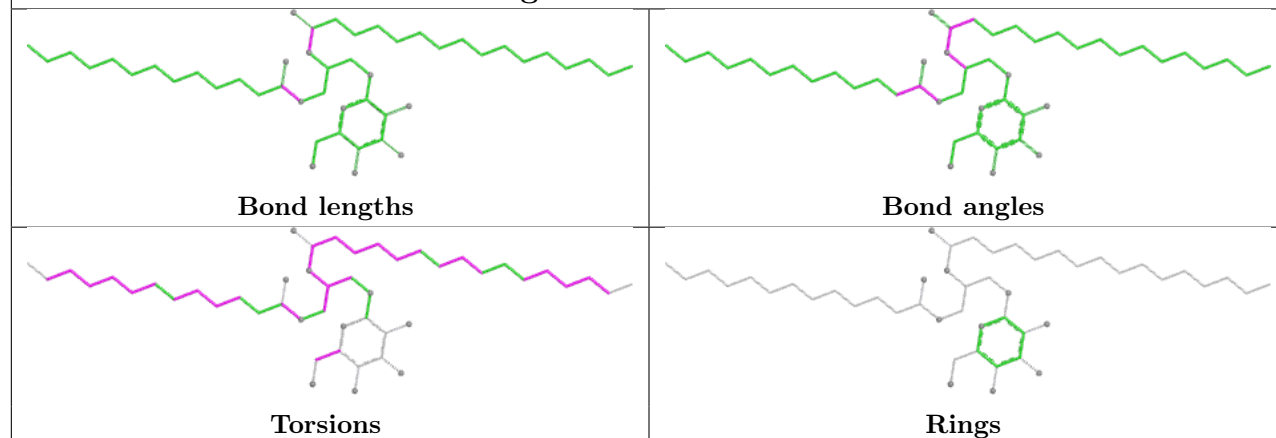
## Ligand CLA C 1037

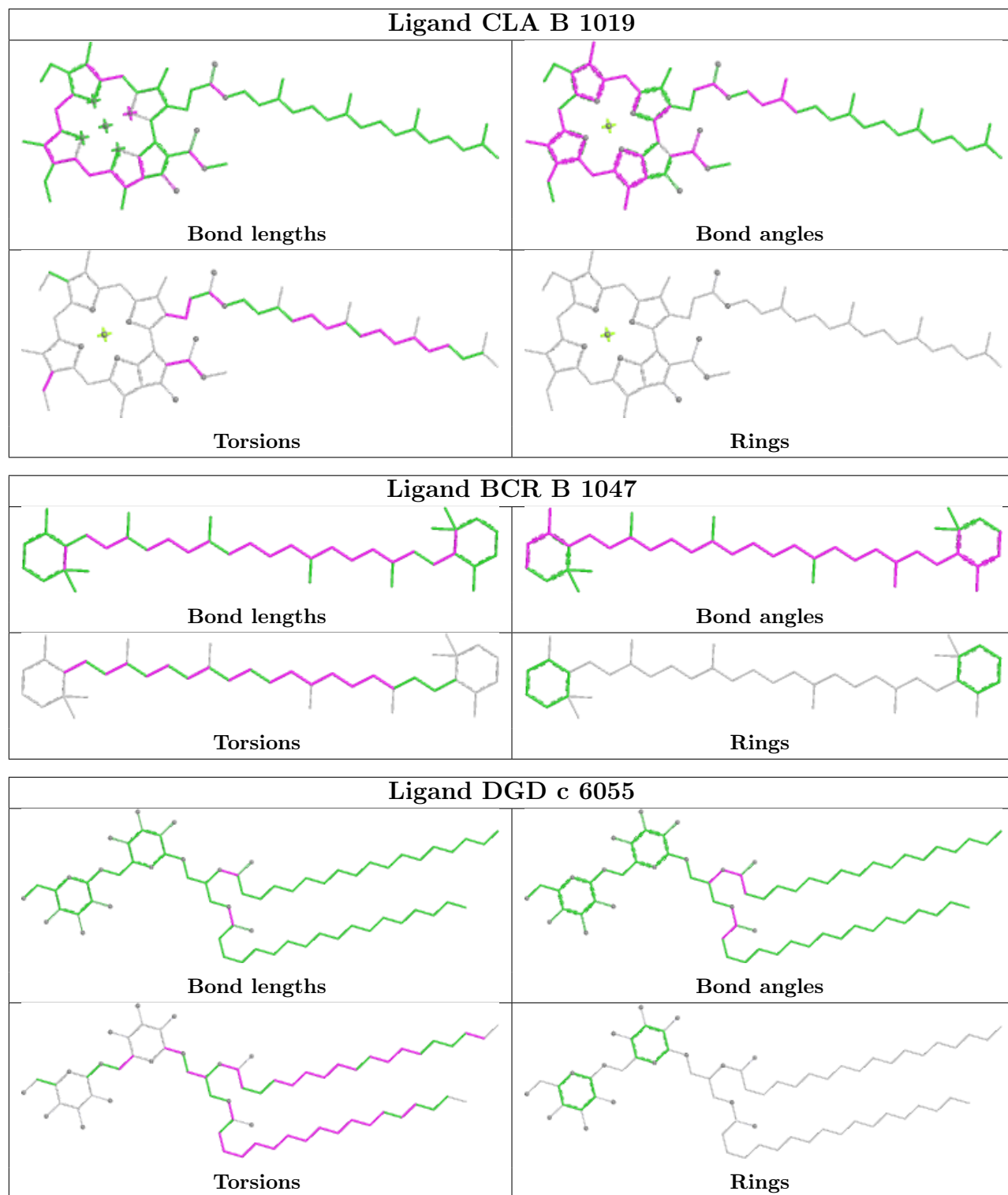


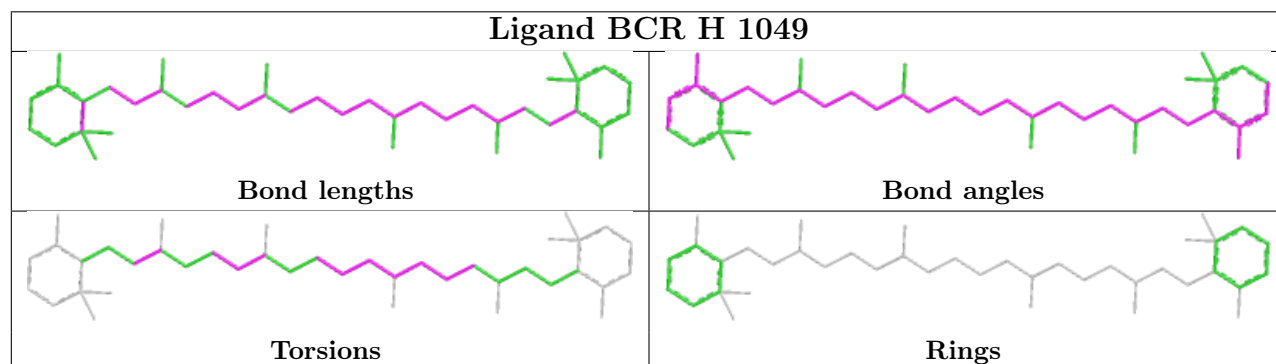
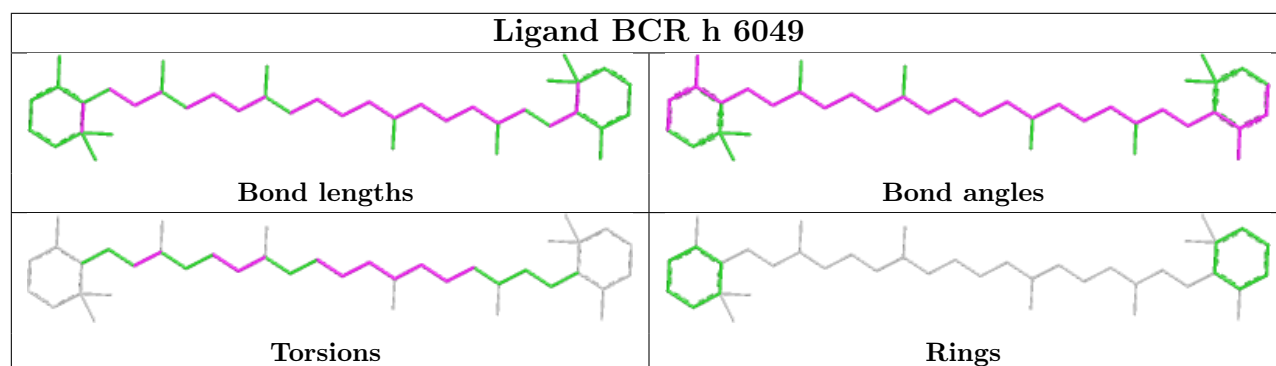
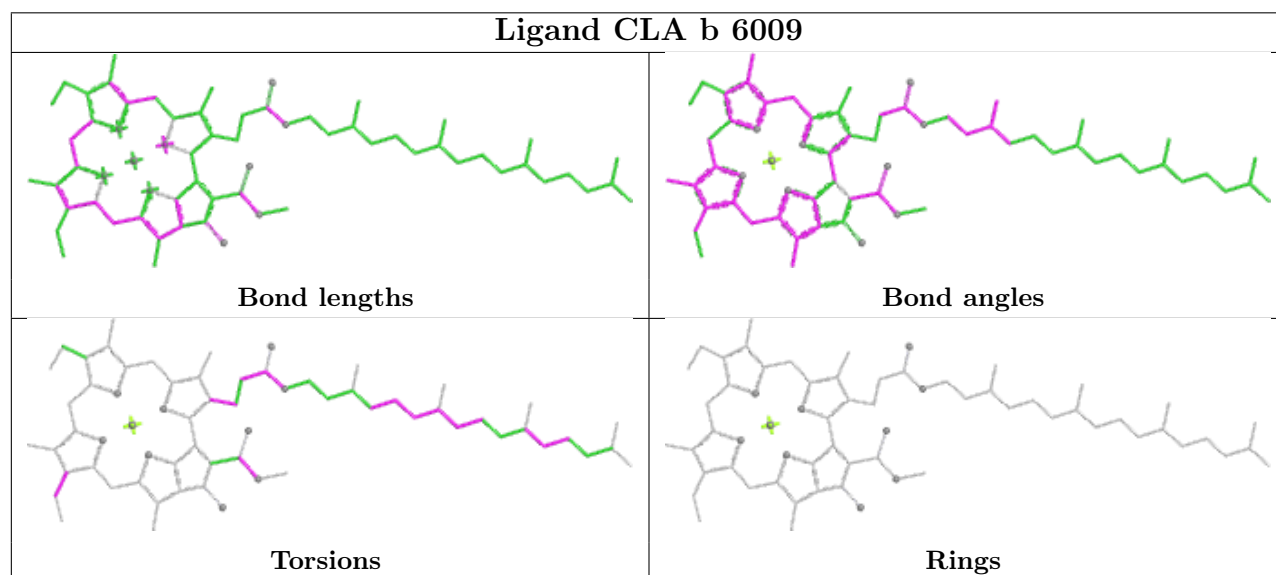
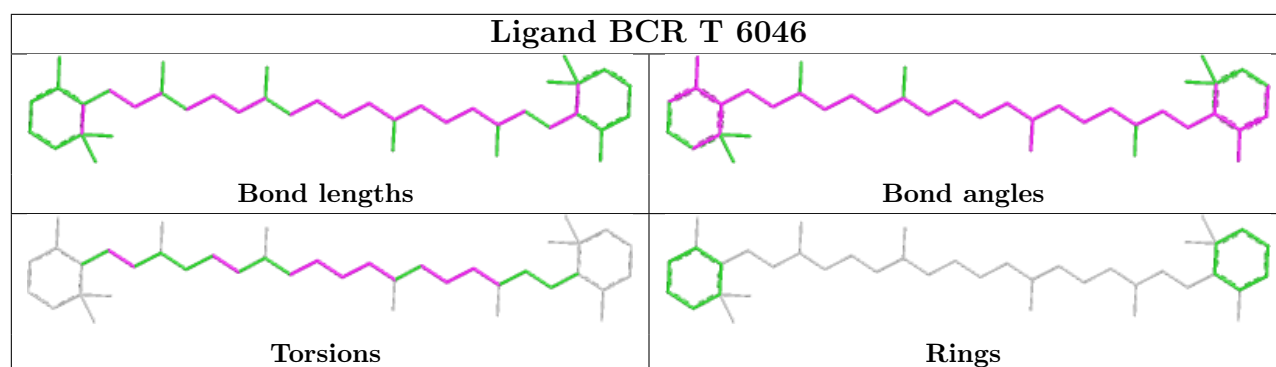
## Ligand CLA B 1024



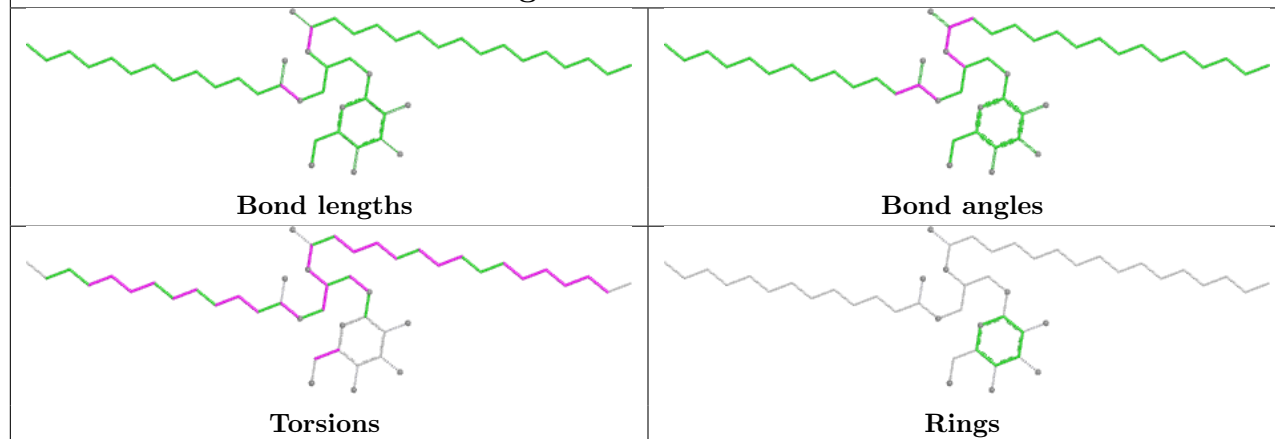
## Ligand MGE b 6060



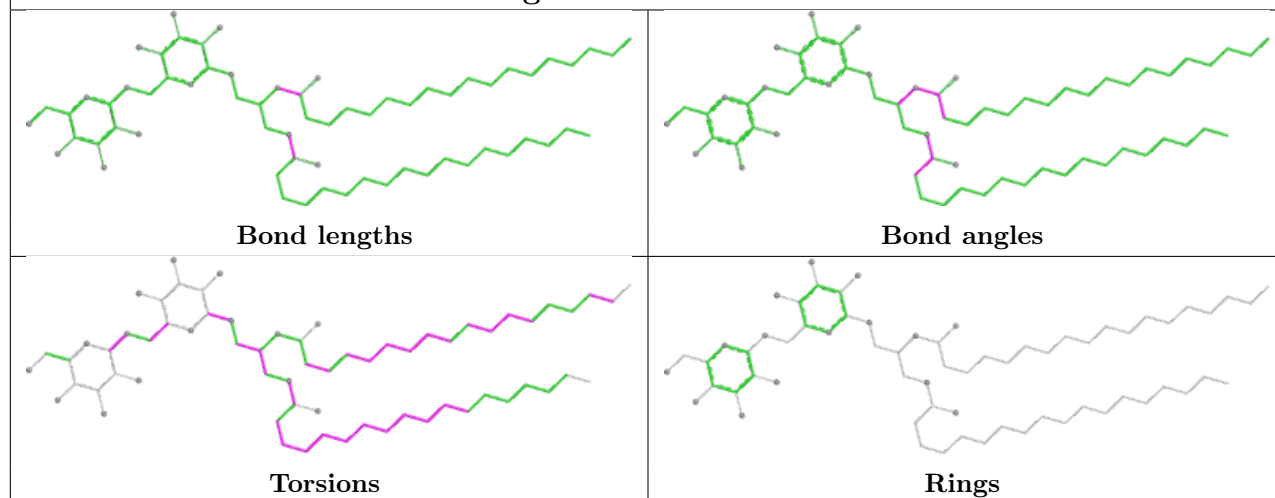




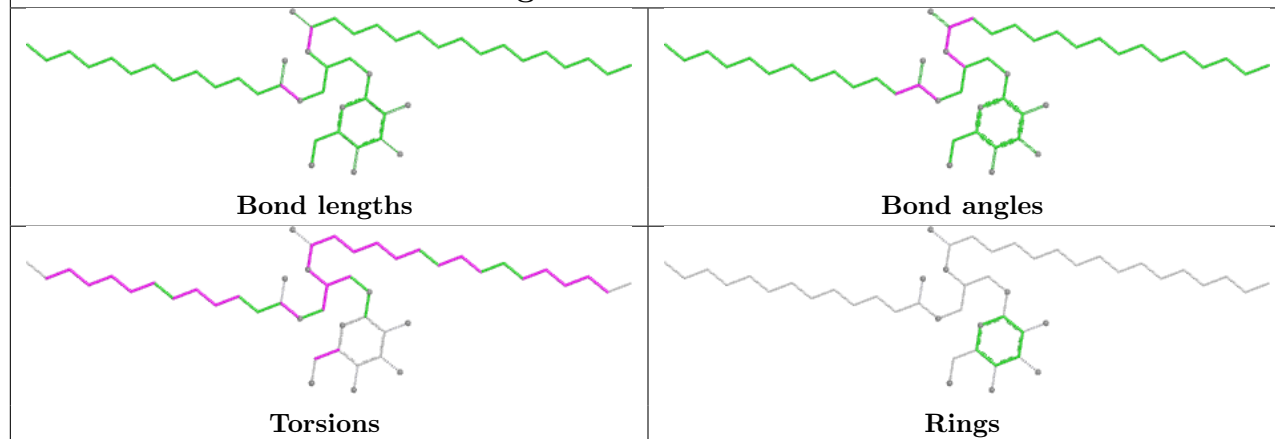
## Ligand MGE L 1061

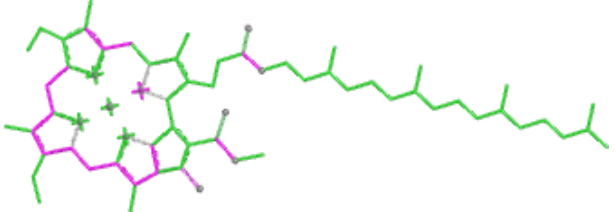
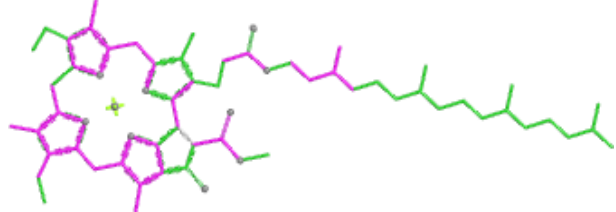
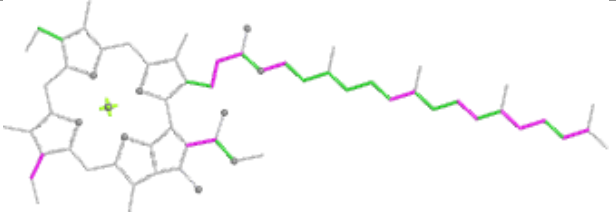
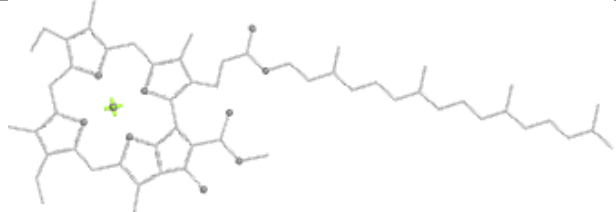
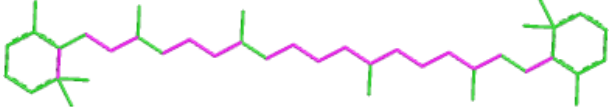
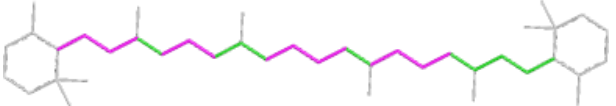
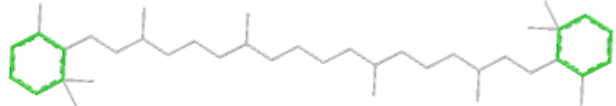
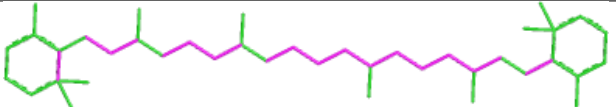
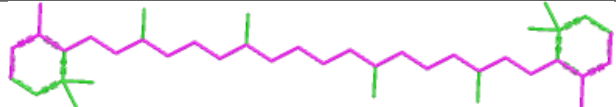
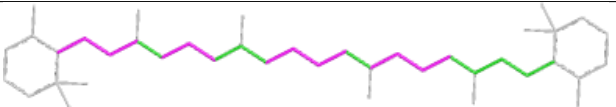
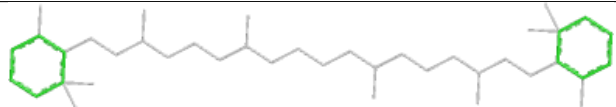


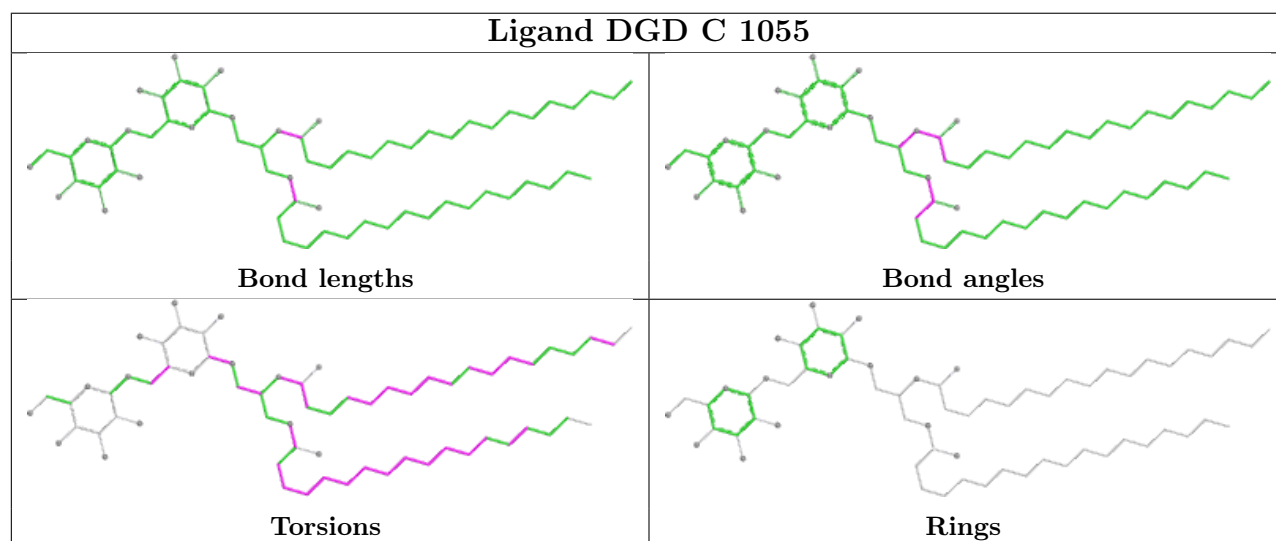
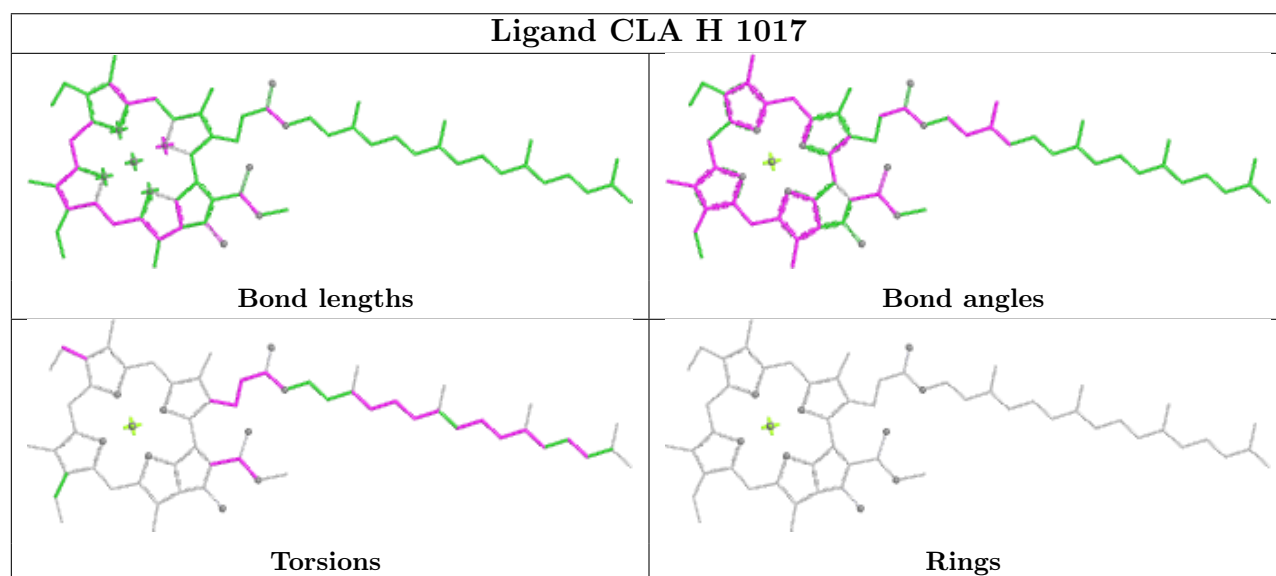
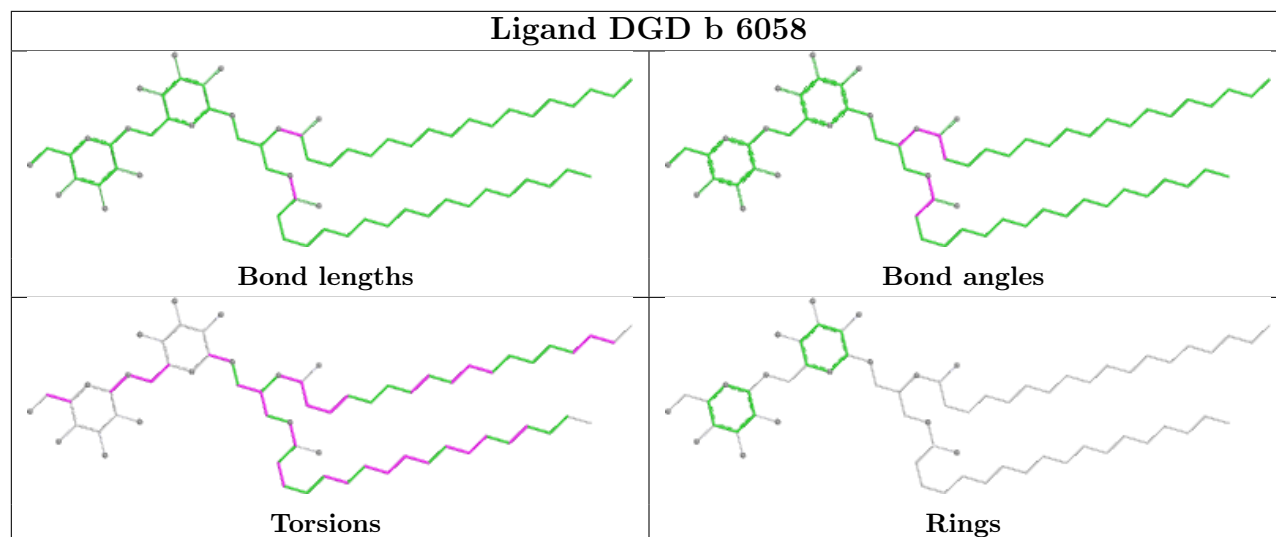
## Ligand DGD c 6057



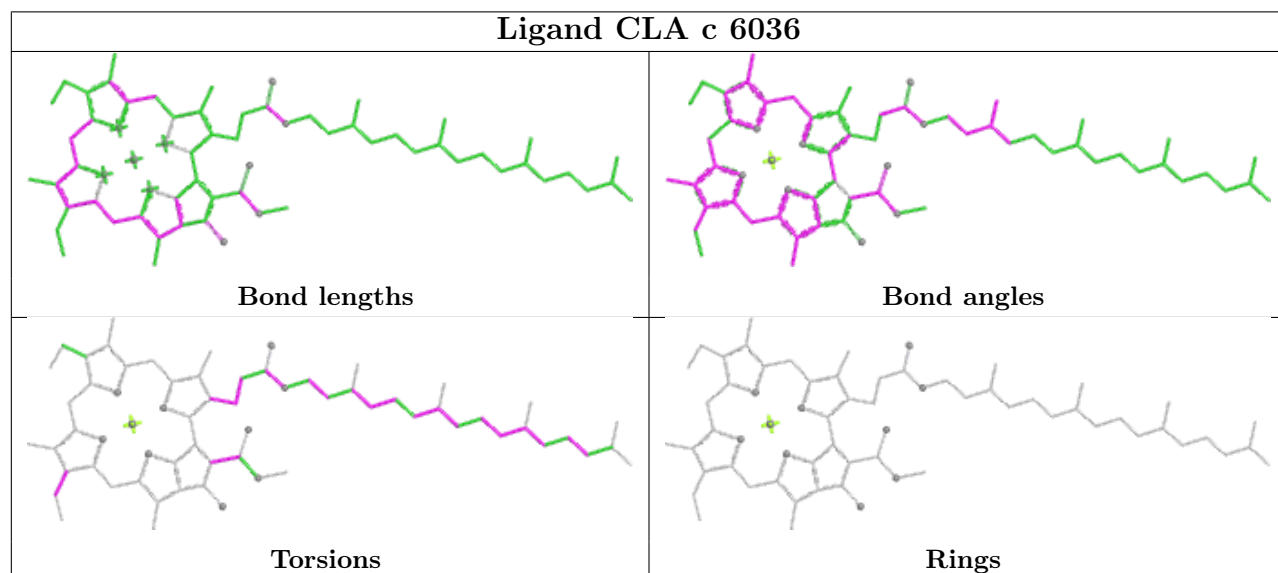
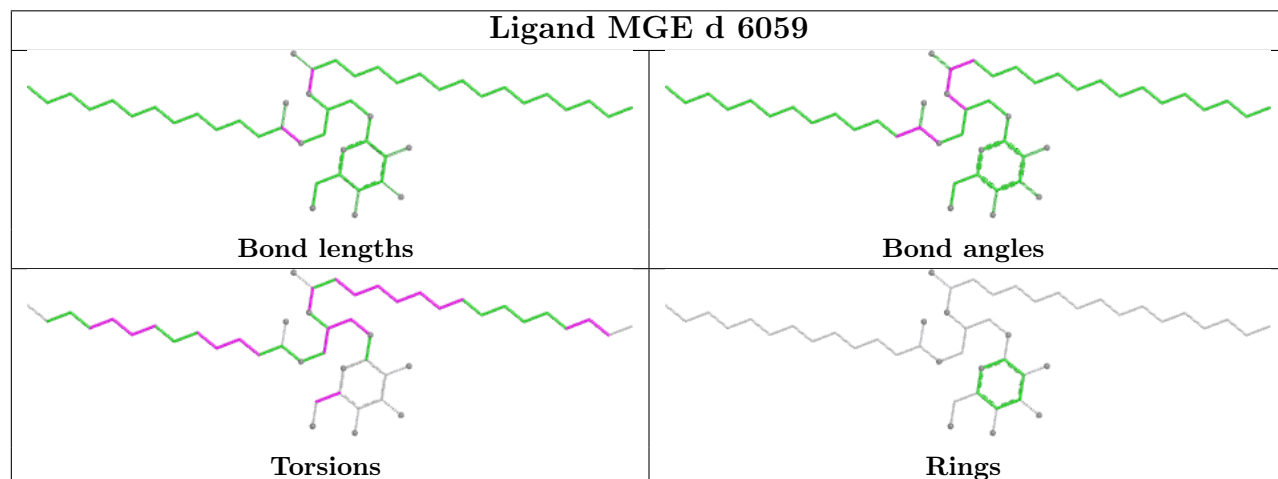
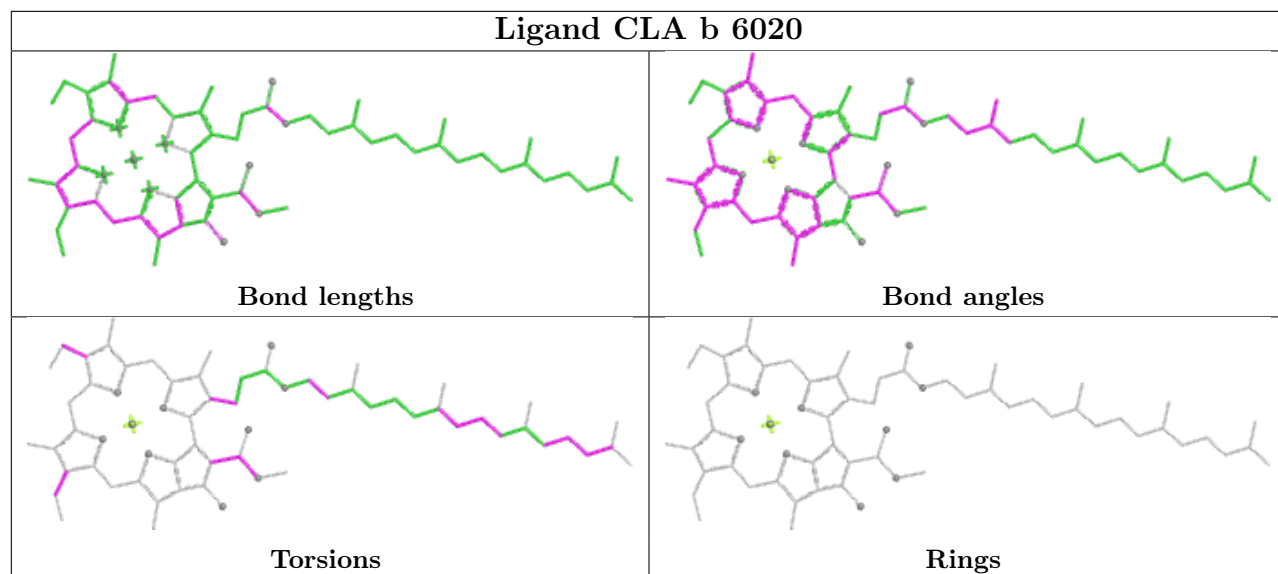
## Ligand MGE B 1060

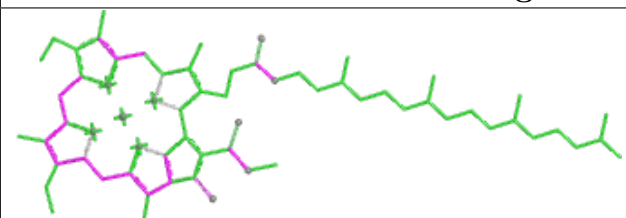
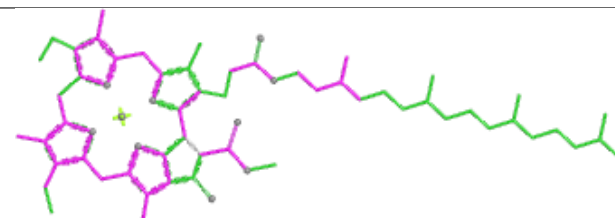
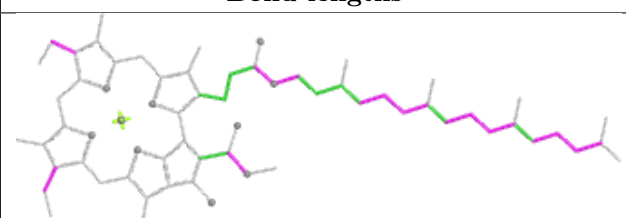
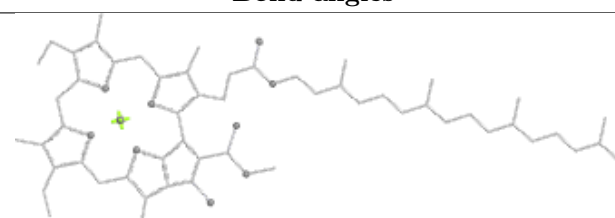


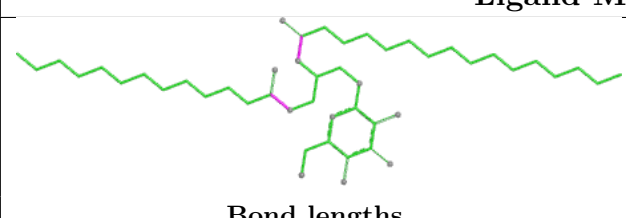
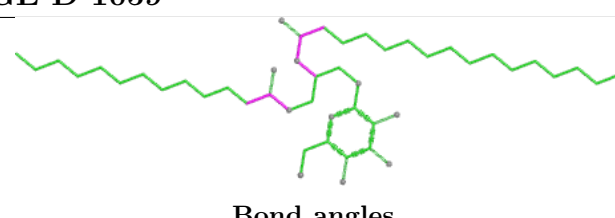
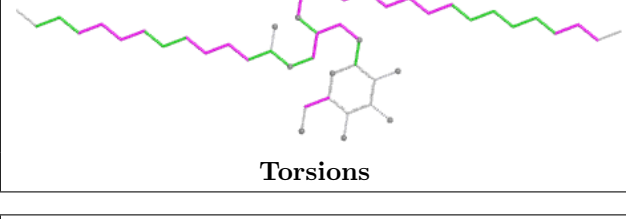
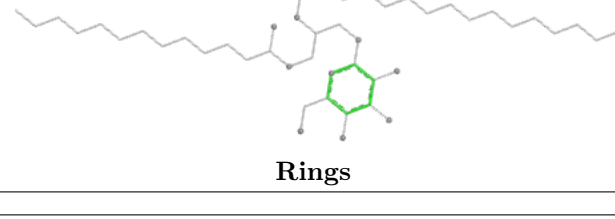
| Ligand CLA c 6031                                                                                       |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR c 6054                                                                                       |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand BCR C 1054                                                                                       |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

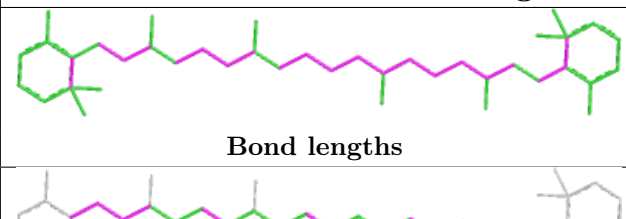
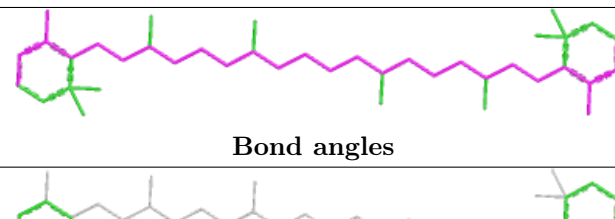
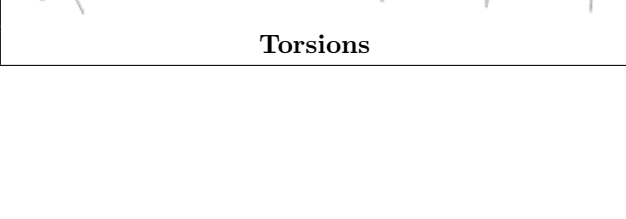
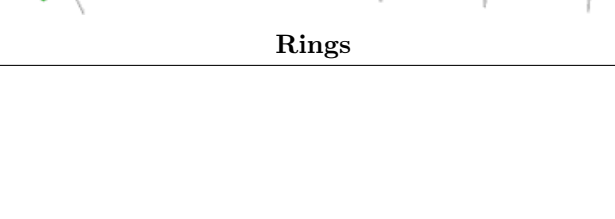


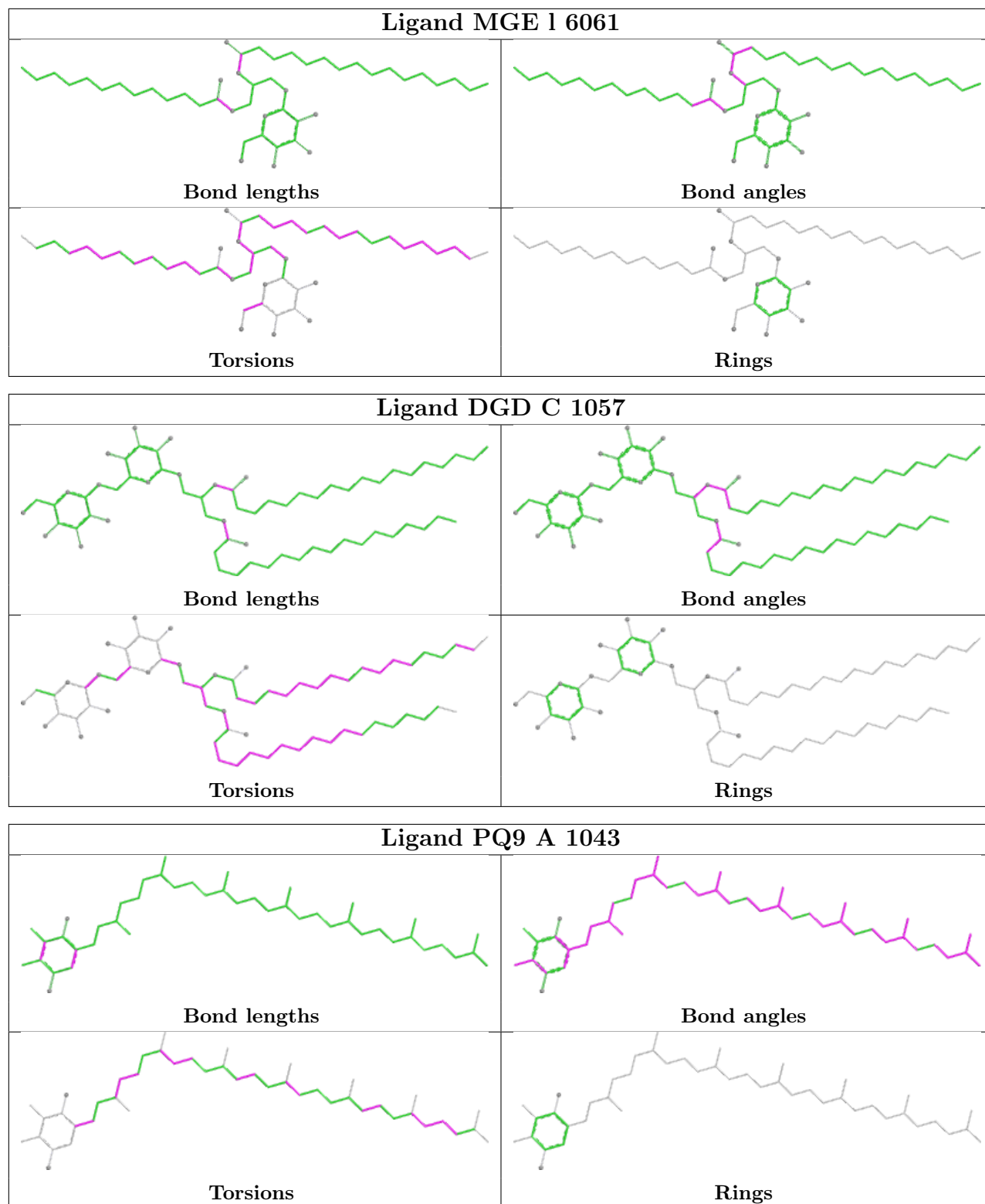


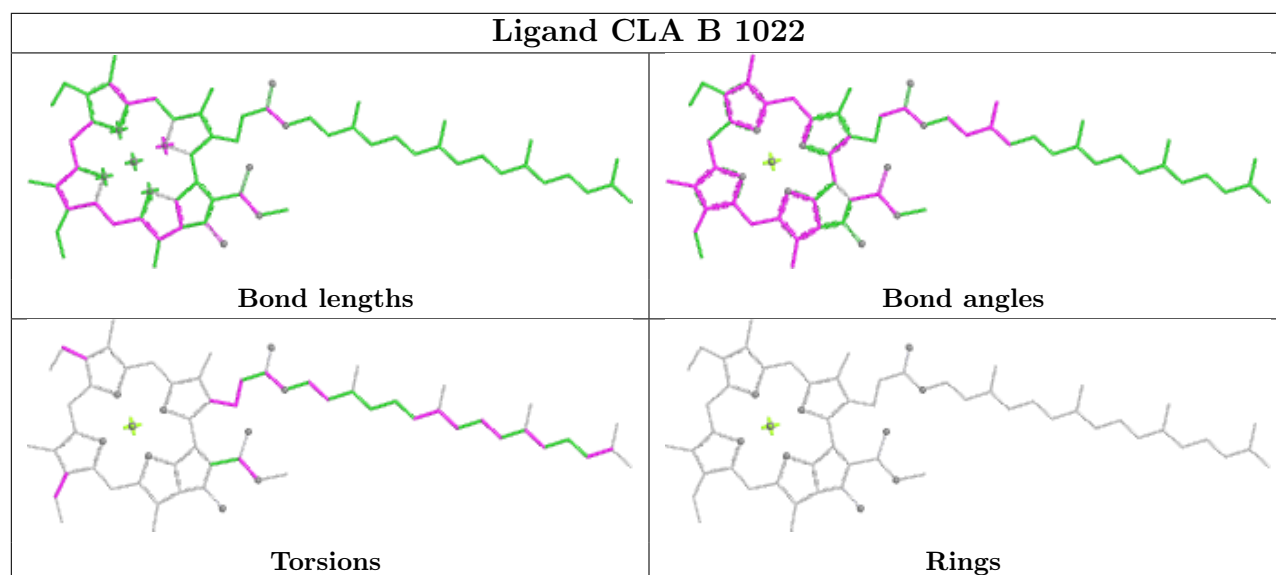
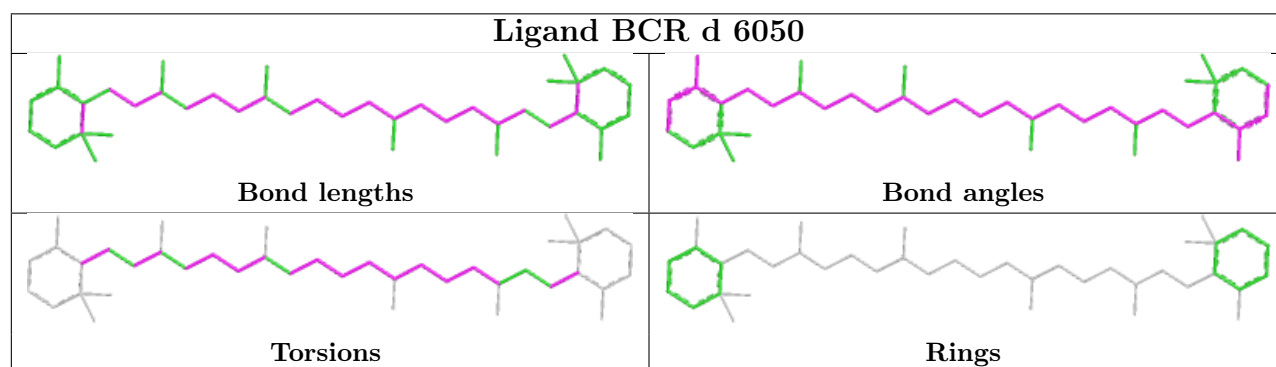
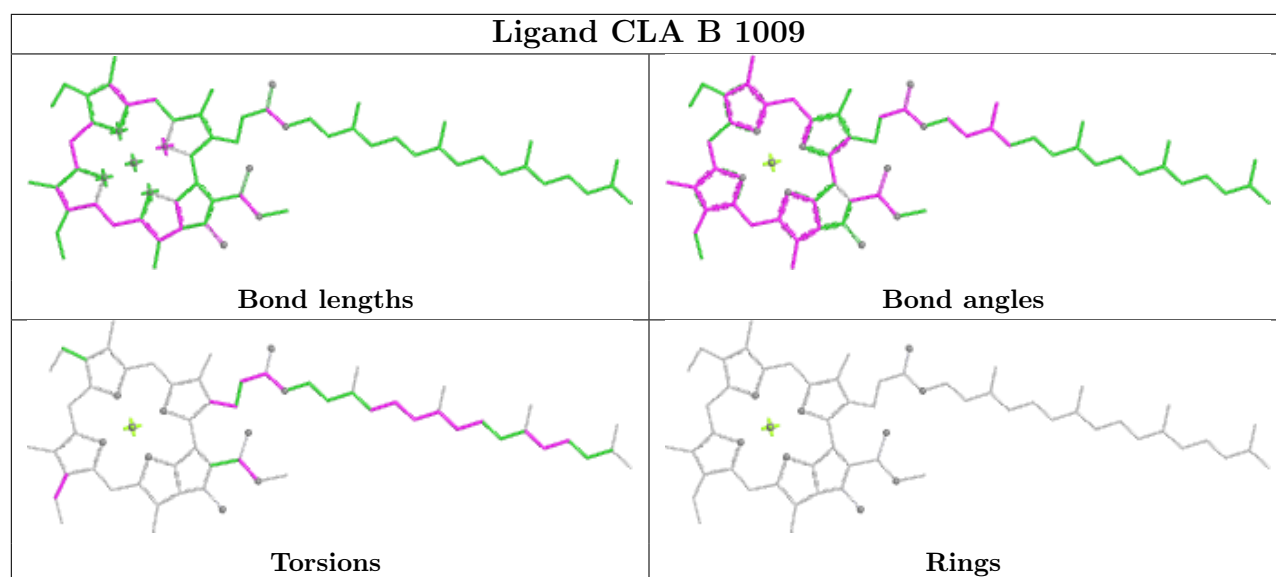


| Ligand CLA b 6016                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

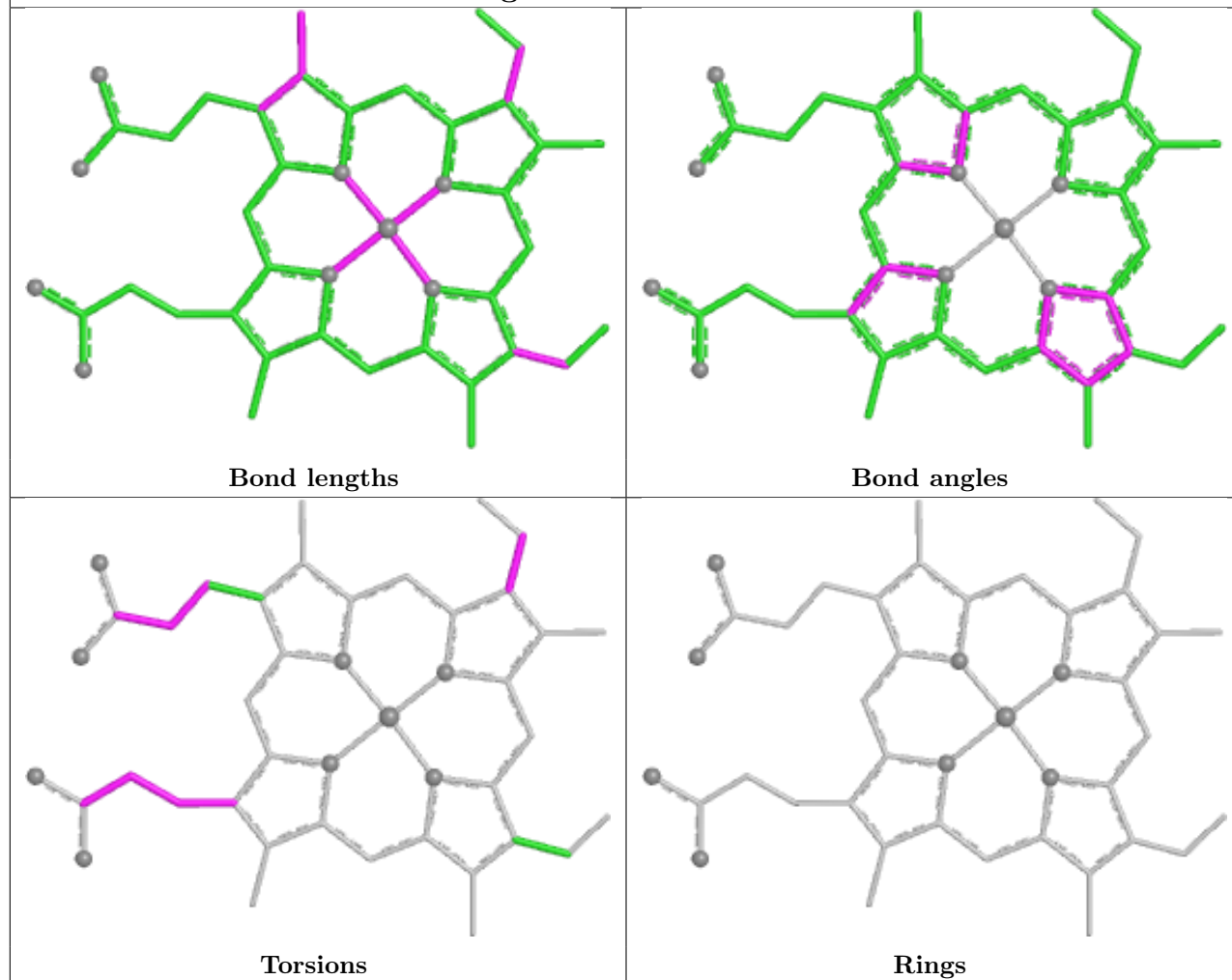
| Ligand MGE D 1059                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand BCR z 6053                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

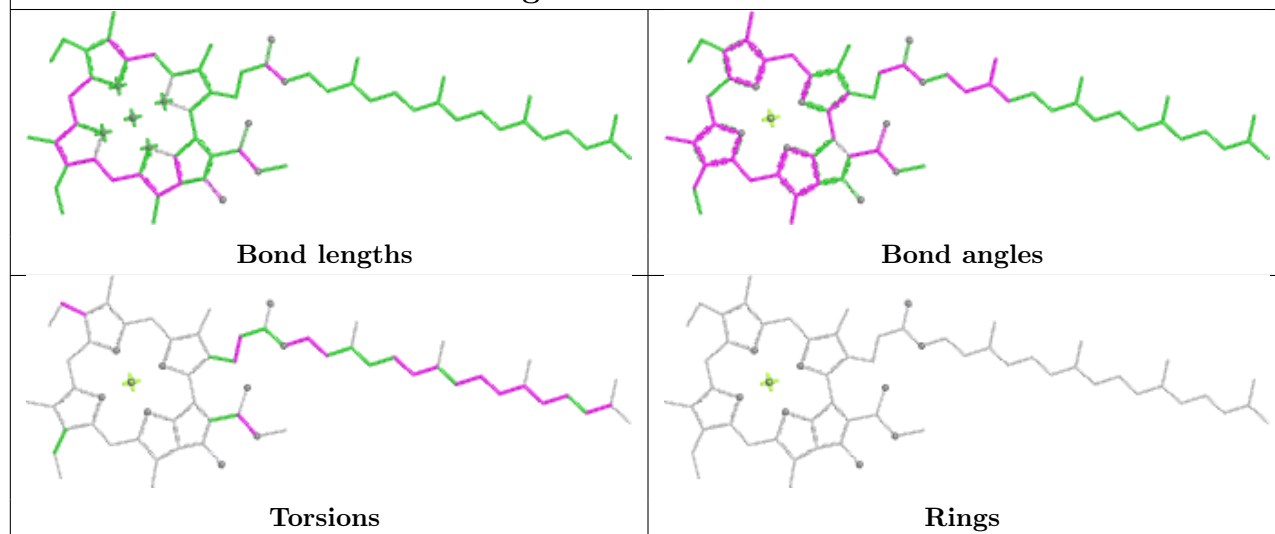


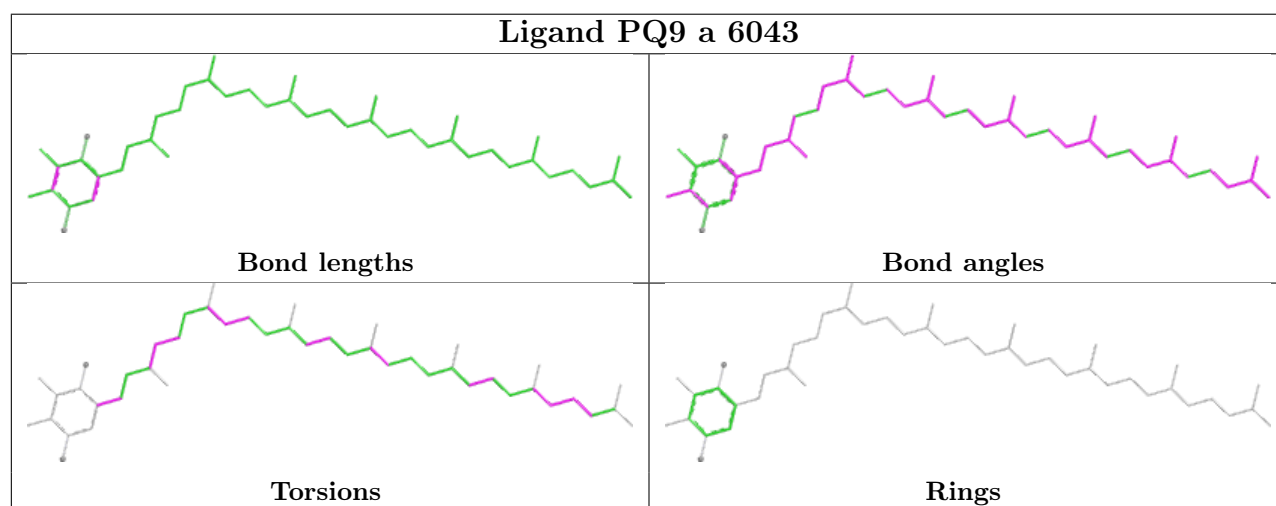
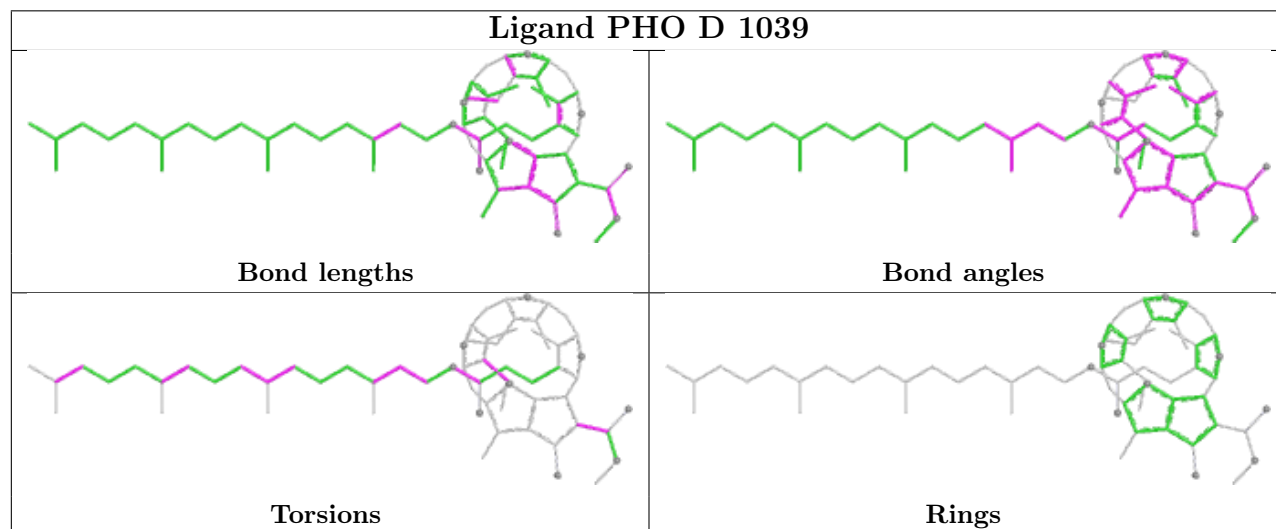
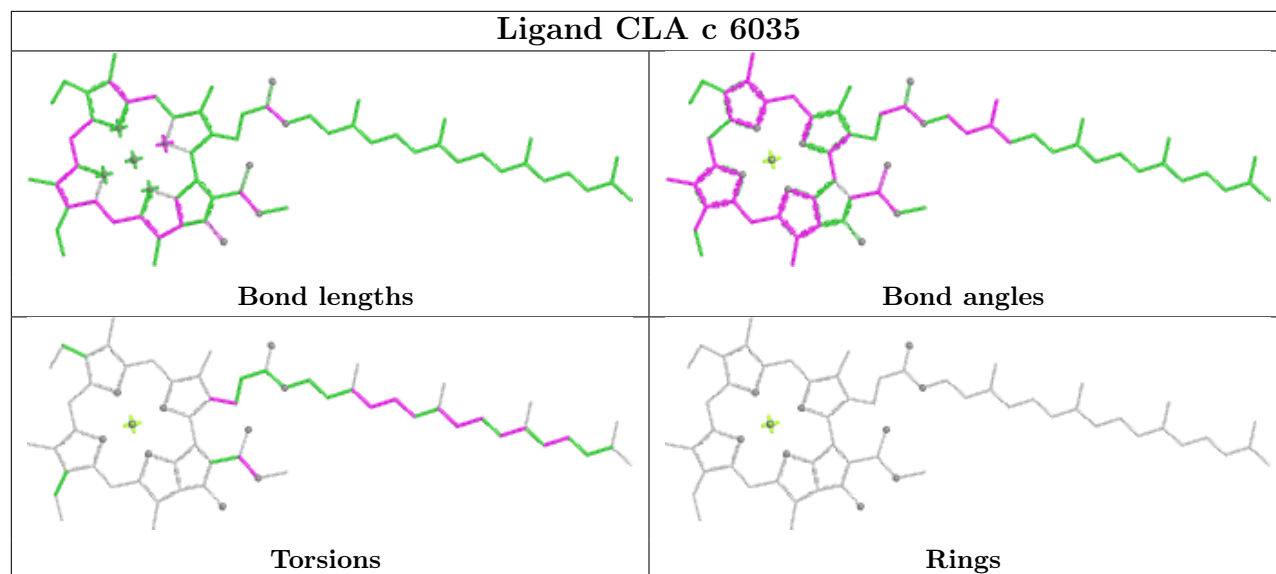


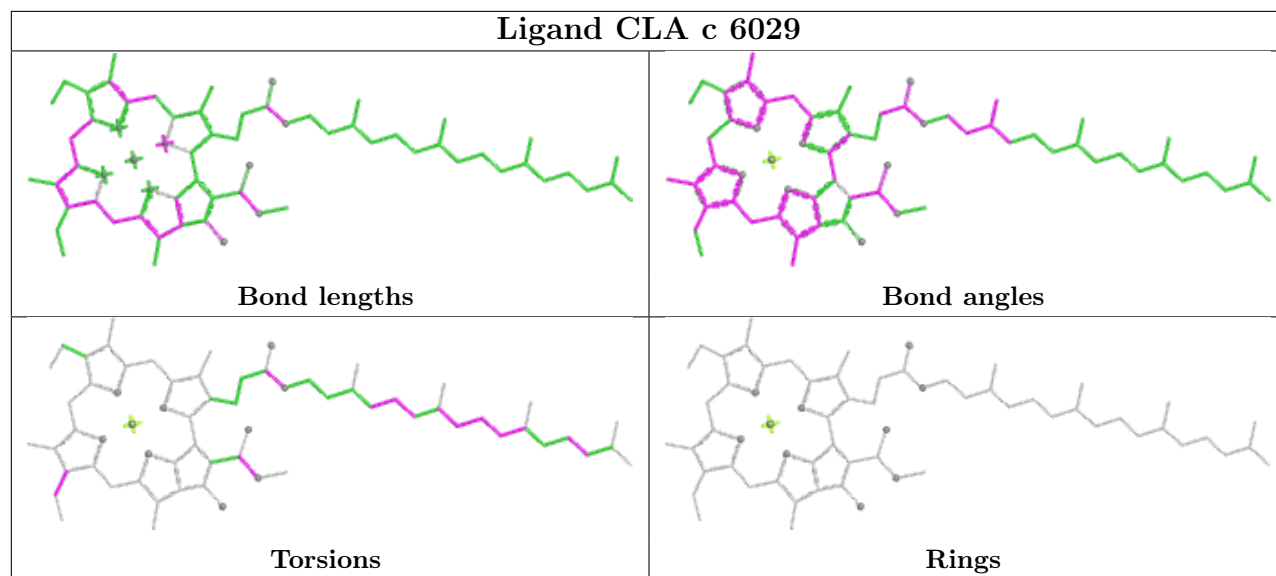
## Ligand HEM F 1040



## Ligand CLA C 1026







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | A     | 335/344 (97%)  | -0.18  | 3 (0%) 81 64 | 135, 156, 186, 200    | 0     |
| 1   | a     | 335/344 (97%)  | -0.30  | 2 (0%) 85 71 | 135, 156, 186, 200    | 0     |
| 2   | B     | 488/488 (100%) | -0.28  | 4 (0%) 82 65 | 133, 156, 180, 191    | 0     |
| 2   | b     | 488/488 (100%) | -0.29  | 2 (0%) 88 75 | 133, 156, 180, 191    | 0     |
| 3   | C     | 447/447 (100%) | -0.24  | 5 (1%) 78 60 | 138, 165, 181, 193    | 0     |
| 3   | c     | 447/447 (100%) | -0.27  | 0 100 100    | 138, 165, 181, 193    | 0     |
| 4   | D     | 340/340 (100%) | -0.24  | 1 (0%) 90 78 | 134, 156, 179, 192    | 0     |
| 4   | d     | 340/340 (100%) | -0.28  | 1 (0%) 90 78 | 134, 156, 179, 192    | 0     |
| 5   | E     | 82/83 (98%)    | -0.35  | 0 100 100    | 153, 172, 191, 198    | 0     |
| 5   | e     | 82/83 (98%)    | -0.41  | 0 100 100    | 153, 172, 191, 198    | 0     |
| 6   | F     | 35/44 (79%)    | -0.47  | 0 100 100    | 153, 167, 187, 191    | 0     |
| 6   | f     | 35/44 (79%)    | -0.32  | 0 100 100    | 153, 167, 187, 191    | 0     |
| 7   | H     | 64/64 (100%)   | -0.36  | 1 (1%) 70 52 | 154, 163, 175, 185    | 0     |
| 7   | h     | 64/64 (100%)   | -0.38  | 0 100 100    | 154, 163, 175, 185    | 0     |
| 8   | I     | 35/35 (100%)   | -0.38  | 0 100 100    | 152, 169, 196, 201    | 0     |
| 8   | i     | 35/35 (100%)   | -0.18  | 0 100 100    | 152, 169, 196, 201    | 0     |
| 9   | J     | 34/40 (85%)    | -0.57  | 0 100 100    | 155, 162, 184, 192    | 0     |
| 9   | j     | 34/40 (85%)    | -0.45  | 0 100 100    | 155, 162, 184, 192    | 0     |
| 10  | K     | 36/36 (100%)   | -0.19  | 1 (2%) 55 40 | 144, 168, 182, 185    | 0     |
| 10  | k     | 36/36 (100%)   | -0.16  | 0 100 100    | 156, 170, 182, 192    | 0     |
| 11  | L     | 37/37 (100%)   | -0.43  | 0 100 100    | 138, 160, 191, 197    | 0     |
| 11  | l     | 37/37 (100%)   | -0.38  | 0 100 100    | 138, 160, 191, 197    | 0     |
| 12  | M     | 36/36 (100%)   | -0.23  | 0 100 100    | 131, 146, 188, 194    | 0     |
| 12  | m     | 36/36 (100%)   | -0.29  | 1 (2%) 55 40 | 131, 146, 188, 194    | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | O     | 242/242 (100%)  | -0.38  | 0 100 100     | 139, 160, 181, 187    | 0     |
| 13  | o     | 242/242 (100%)  | -0.38  | 0 100 100     | 139, 160, 181, 187    | 0     |
| 14  | T     | 30/30 (100%)    | -0.58  | 0 100 100     | 124, 143, 186, 191    | 0     |
| 14  | t     | 30/30 (100%)    | -0.39  | 0 100 100     | 131, 143, 186, 191    | 0     |
| 15  | U     | 98/98 (100%)    | -0.46  | 0 100 100     | 139, 155, 165, 173    | 0     |
| 15  | u     | 98/98 (100%)    | -0.52  | 0 100 100     | 139, 155, 165, 173    | 0     |
| 16  | V     | 137/137 (100%)  | -0.17  | 3 (2%) 62 46  | 144, 162, 173, 178    | 0     |
| 16  | v     | 137/137 (100%)  | -0.33  | 0 100 100     | 144, 162, 173, 178    | 0     |
| 17  | X     | 34/34 (100%)    | -0.25  | 1 (2%) 53 39  | 173, 181, 198, 201    | 0     |
| 17  | x     | 34/34 (100%)    | -0.39  | 0 100 100     | 173, 181, 198, 201    | 0     |
| 18  | Y     | 28/28 (100%)    | -0.18  | 0 100 100     | 187, 199, 208, 210    | 0     |
| 18  | y     | 28/28 (100%)    | -0.27  | 0 100 100     | 187, 199, 208, 210    | 0     |
| 19  | N     | 0/23            | -      | -             | -                     | -     |
| 19  | n     | 0/23            | -      | -             | -                     | -     |
| 20  | Z     | 62/62 (100%)    | -0.45  | 0 100 100     | 159, 173, 188, 196    | 0     |
| 20  | z     | 62/62 (100%)    | -0.33  | 1 (1%) 70 52  | 159, 173, 188, 196    | 0     |
| All | All   | 5200/5296 (98%) | -0.30  | 26 (0%) 87 73 | 124, 161, 185, 210    | 0     |

All (26) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 279  | ARG  | 6.3  |
| 1   | a     | 5279 | ARG  | 6.1  |
| 3   | C     | 44   | ASN  | 3.9  |
| 2   | B     | 166  | MET  | 3.2  |
| 3   | C     | 45   | LEU  | 3.1  |
| 16  | V     | 63   | CYS  | 2.8  |
| 16  | V     | 78   | LEU  | 2.8  |
| 1   | a     | 5205 | VAL  | 2.7  |
| 10  | K     | 37   | PHE  | 2.7  |
| 2   | B     | 190  | PHE  | 2.5  |
| 1   | A     | 209  | ALA  | 2.5  |
| 1   | A     | 250  | ALA  | 2.5  |
| 16  | V     | 139  | VAL  | 2.5  |
| 2   | b     | 5068 | ARG  | 2.5  |
| 17  | X     | 44   | ASP  | 2.4  |
| 2   | b     | 5031 | ALA  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 86   | LEU  | 2.3  |
| 12  | m     | 5008 | PHE  | 2.2  |
| 7   | H     | 62   | TRP  | 2.2  |
| 3   | C     | 348  | GLU  | 2.2  |
| 4   | d     | 5136 | VAL  | 2.2  |
| 3   | C     | 234  | VAL  | 2.1  |
| 2   | B     | 68   | ARG  | 2.1  |
| 4   | D     | 291  | LEU  | 2.1  |
| 20  | z     | 5042 | LEU  | 2.0  |
| 2   | B     | 379  | ALA  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 27  | IOD  | D     | 1068 | 1/1   | 0.20 | 0.60 | 198,198,198,198            | 0     |
| 27  | IOD  | B     | 1067 | 1/1   | 0.47 | 0.43 | 198,198,198,198            | 0     |
| 22  | CLA  | K     | 1034 | 65/65 | 0.56 | 0.18 | 138,189,216,216            | 0     |
| 26  | LHG  | a     | 6063 | 49/49 | 0.57 | 0.19 | 199,213,216,216            | 0     |
| 22  | CLA  | B     | 1009 | 65/65 | 0.57 | 0.17 | 143,192,213,213            | 0     |
| 26  | LHG  | A     | 1063 | 49/49 | 0.57 | 0.20 | 199,213,216,216            | 0     |
| 22  | CLA  | k     | 6034 | 65/65 | 0.63 | 0.18 | 138,189,216,216            | 0     |
| 25  | BCR  | T     | 6048 | 40/40 | 0.63 | 0.16 | 179,184,203,204            | 0     |
| 27  | IOD  | b     | 6067 | 1/1   | 0.67 | 0.42 | 199,199,199,199            | 0     |
| 25  | BCR  | A     | 1044 | 40/40 | 0.70 | 0.18 | 155,177,185,185            | 0     |
| 25  | BCR  | B     | 1048 | 40/40 | 0.70 | 0.16 | 179,184,203,204            | 0     |
| 25  | BCR  | b     | 6047 | 40/40 | 0.71 | 0.13 | 155,171,200,202            | 0     |
| 22  | CLA  | b     | 6009 | 65/65 | 0.71 | 0.14 | 143,192,213,213            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22  | CLA  | c     | 6037 | 65/65 | 0.71 | 0.13 | 201,211,214,216             | 0     |
| 22  | CLA  | c     | 6027 | 65/65 | 0.72 | 0.17 | 192,198,204,216             | 0     |
| 29  | DGD  | C     | 1056 | 66/66 | 0.72 | 0.14 | 190,201,216,216             | 0     |
| 27  | IOD  | T     | 1066 | 1/1   | 0.73 | 0.23 | 199,199,199,199             | 0     |
| 22  | CLA  | C     | 1027 | 65/65 | 0.73 | 0.19 | 192,198,204,216             | 0     |
| 25  | BCR  | c     | 6054 | 40/40 | 0.73 | 0.19 | 197,201,216,216             | 0     |
| 25  | BCR  | k     | 6052 | 40/40 | 0.75 | 0.27 | 191,195,202,203             | 0     |
| 27  | IOD  | d     | 6068 | 1/1   | 0.75 | 0.39 | 199,199,199,199             | 0     |
| 22  | CLA  | d     | 6008 | 65/65 | 0.75 | 0.16 | 184,188,216,216             | 0     |
| 25  | BCR  | Z     | 1053 | 40/40 | 0.76 | 0.15 | 190,214,216,216             | 0     |
| 22  | CLA  | c     | 6026 | 65/65 | 0.77 | 0.16 | 138,171,178,183             | 0     |
| 25  | BCR  | z     | 6053 | 40/40 | 0.77 | 0.13 | 190,214,216,216             | 0     |
| 25  | BCR  | b     | 6045 | 40/40 | 0.77 | 0.19 | 163,196,216,216             | 0     |
| 25  | BCR  | C     | 1054 | 40/40 | 0.77 | 0.22 | 197,201,216,216             | 0     |
| 28  | MGE  | d     | 6062 | 48/48 | 0.77 | 0.19 | 187,202,208,210             | 0     |
| 25  | BCR  | B     | 1047 | 40/40 | 0.77 | 0.13 | 155,171,200,202             | 0     |
| 29  | DGD  | c     | 6056 | 66/66 | 0.77 | 0.12 | 190,201,216,216             | 0     |
| 22  | CLA  | b     | 6014 | 65/65 | 0.78 | 0.16 | 178,187,197,216             | 0     |
| 28  | MGE  | B     | 1060 | 48/48 | 0.79 | 0.20 | 186,199,213,216             | 0     |
| 28  | MGE  | D     | 1059 | 48/48 | 0.79 | 0.16 | 179,190,215,216             | 0     |
| 25  | BCR  | T     | 6046 | 40/40 | 0.79 | 0.15 | 179,185,188,189             | 0     |
| 22  | CLA  | C     | 1037 | 65/65 | 0.79 | 0.13 | 201,211,214,216             | 0     |
| 25  | BCR  | d     | 6050 | 40/40 | 0.79 | 0.17 | 184,193,198,199             | 0     |
| 22  | CLA  | B     | 1014 | 65/65 | 0.80 | 0.14 | 178,187,197,216             | 0     |
| 28  | MGE  | d     | 6059 | 48/48 | 0.80 | 0.15 | 179,190,215,216             | 0     |
| 25  | BCR  | h     | 6049 | 40/40 | 0.80 | 0.17 | 177,182,188,189             | 0     |
| 25  | BCR  | D     | 1050 | 40/40 | 0.80 | 0.18 | 184,193,198,199             | 0     |
| 25  | BCR  | K     | 1051 | 40/40 | 0.80 | 0.23 | 192,202,210,210             | 0     |
| 25  | BCR  | a     | 6044 | 40/40 | 0.81 | 0.15 | 155,177,185,185             | 0     |
| 24  | PQ9  | A     | 1043 | 45/45 | 0.81 | 0.26 | 171,172,193,197             | 30    |
| 22  | CLA  | b     | 6021 | 65/65 | 0.81 | 0.15 | 154,164,172,176             | 0     |
| 28  | MGE  | b     | 6060 | 48/48 | 0.82 | 0.19 | 186,199,213,216             | 0     |
| 22  | CLA  | d     | 6005 | 65/65 | 0.82 | 0.17 | 135,162,169,173             | 0     |
| 24  | PQ9  | d     | 6042 | 45/45 | 0.82 | 0.24 | 171,173,185,187             | 0     |
| 28  | MGE  | l     | 6061 | 48/48 | 0.82 | 0.17 | 177,191,195,199             | 0     |
| 22  | CLA  | c     | 6035 | 65/65 | 0.82 | 0.19 | 189,202,210,216             | 0     |
| 29  | DGD  | C     | 1057 | 66/66 | 0.82 | 0.15 | 177,190,206,207             | 0     |
| 22  | CLA  | C     | 1030 | 65/65 | 0.82 | 0.13 | 185,197,216,216             | 0     |
| 29  | DGD  | c     | 6057 | 66/66 | 0.82 | 0.15 | 177,190,206,207             | 0     |
| 22  | CLA  | B     | 1021 | 65/65 | 0.83 | 0.12 | 154,164,172,176             | 0     |
| 23  | PHO  | D     | 1039 | 64/64 | 0.83 | 0.16 | 184,187,196,198             | 0     |
| 22  | CLA  | D     | 1005 | 65/65 | 0.83 | 0.15 | 135,162,169,173             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 28  | MGE  | L     | 1061 | 48/48 | 0.83 | 0.19 | 177,191,195,199             | 0     |
| 22  | CLA  | b     | 6015 | 65/65 | 0.84 | 0.13 | 177,182,185,216             | 0     |
| 25  | BCR  | H     | 1049 | 40/40 | 0.84 | 0.17 | 177,182,188,189             | 0     |
| 29  | DGD  | c     | 6055 | 66/66 | 0.84 | 0.17 | 184,192,202,203             | 0     |
| 28  | MGE  | D     | 1062 | 48/48 | 0.84 | 0.19 | 187,202,208,210             | 0     |
| 22  | CLA  | C     | 1036 | 65/65 | 0.84 | 0.14 | 186,190,203,216             | 0     |
| 25  | BCR  | B     | 1045 | 40/40 | 0.85 | 0.15 | 163,196,216,216             | 0     |
| 22  | CLA  | C     | 1026 | 65/65 | 0.85 | 0.16 | 138,171,178,183             | 0     |
| 25  | BCR  | k     | 6051 | 40/40 | 0.85 | 0.18 | 192,202,210,210             | 0     |
| 22  | CLA  | b     | 6024 | 65/65 | 0.85 | 0.13 | 165,193,197,198             | 0     |
| 22  | CLA  | c     | 6025 | 65/65 | 0.85 | 0.11 | 156,187,191,194             | 0     |
| 22  | CLA  | c     | 6036 | 65/65 | 0.85 | 0.12 | 186,190,203,216             | 0     |
| 24  | PQ9  | a     | 6043 | 45/45 | 0.86 | 0.23 | 171,172,193,197             | 30    |
| 22  | CLA  | C     | 1028 | 65/65 | 0.86 | 0.15 | 178,182,201,202             | 0     |
| 22  | CLA  | c     | 6032 | 65/65 | 0.86 | 0.14 | 186,189,200,216             | 0     |
| 22  | CLA  | B     | 1024 | 65/65 | 0.87 | 0.12 | 165,193,197,198             | 0     |
| 22  | CLA  | b     | 6019 | 65/65 | 0.87 | 0.12 | 167,172,175,180             | 0     |
| 29  | DGD  | C     | 1055 | 66/66 | 0.87 | 0.19 | 184,192,202,203             | 0     |
| 22  | CLA  | a     | 6007 | 65/65 | 0.87 | 0.17 | 129,174,204,205             | 0     |
| 22  | CLA  | C     | 1025 | 65/65 | 0.88 | 0.12 | 156,187,191,194             | 0     |
| 25  | BCR  | t     | 1046 | 40/40 | 0.88 | 0.12 | 179,185,188,189             | 0     |
| 29  | DGD  | B     | 1058 | 66/66 | 0.88 | 0.20 | 175,188,196,203             | 0     |
| 22  | CLA  | C     | 1032 | 65/65 | 0.88 | 0.16 | 184,188,192,216             | 0     |
| 22  | CLA  | b     | 6012 | 65/65 | 0.88 | 0.14 | 160,167,172,174             | 0     |
| 23  | PHO  | a     | 6038 | 64/64 | 0.88 | 0.14 | 166,176,178,181             | 0     |
| 29  | DGD  | b     | 6058 | 66/66 | 0.88 | 0.20 | 175,188,196,203             | 0     |
| 23  | PHO  | d     | 6039 | 64/64 | 0.88 | 0.12 | 184,187,196,198             | 0     |
| 22  | CLA  | C     | 1029 | 65/65 | 0.88 | 0.14 | 177,187,190,201             | 0     |
| 25  | BCR  | C     | 1052 | 40/40 | 0.88 | 0.29 | 191,195,202,203             | 0     |
| 22  | CLA  | a     | 6003 | 65/65 | 0.89 | 0.17 | 160,169,175,212             | 0     |
| 22  | CLA  | c     | 6031 | 65/65 | 0.89 | 0.16 | 181,185,202,216             | 0     |
| 22  | CLA  | b     | 6022 | 65/65 | 0.89 | 0.13 | 138,180,198,200             | 0     |
| 22  | CLA  | D     | 1008 | 65/65 | 0.89 | 0.13 | 184,188,216,216             | 0     |
| 22  | CLA  | B     | 1011 | 65/65 | 0.89 | 0.12 | 168,178,184,188             | 0     |
| 22  | CLA  | b     | 6011 | 65/65 | 0.89 | 0.15 | 168,178,184,188             | 0     |
| 31  | HEM  | f     | 6040 | 43/43 | 0.89 | 0.20 | 186,215,216,216             | 0     |
| 22  | CLA  | a     | 6006 | 65/65 | 0.90 | 0.11 | 166,181,211,213             | 0     |
| 24  | PQ9  | D     | 1042 | 45/45 | 0.90 | 0.19 | 171,173,185,187             | 0     |
| 22  | CLA  | c     | 6028 | 65/65 | 0.90 | 0.13 | 178,182,201,202             | 0     |
| 22  | CLA  | c     | 6029 | 65/65 | 0.90 | 0.13 | 177,187,190,201             | 0     |
| 22  | CLA  | h     | 6017 | 65/65 | 0.90 | 0.14 | 169,197,201,208             | 0     |
| 22  | CLA  | B     | 1019 | 65/65 | 0.90 | 0.13 | 167,172,175,180             | 0     |

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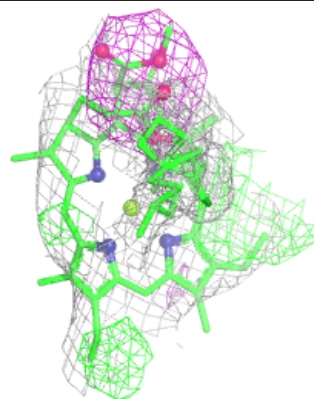
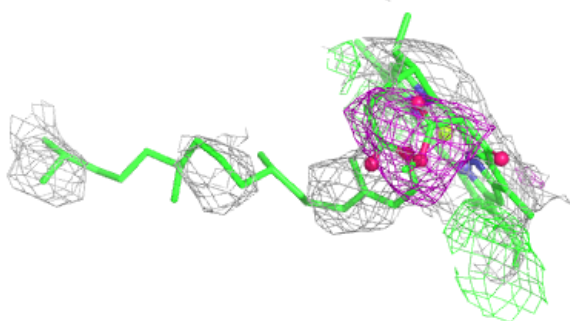
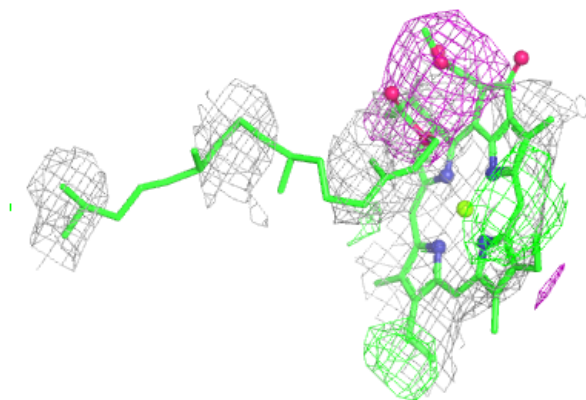
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | PHO  | A     | 1038 | 64/64 | 0.90 | 0.13 | 166,176,178,181             | 0     |
| 22  | CLA  | A     | 1006 | 65/65 | 0.90 | 0.14 | 166,181,211,213             | 0     |
| 22  | CLA  | b     | 6016 | 65/65 | 0.90 | 0.12 | 130,172,175,180             | 0     |
| 22  | CLA  | C     | 1035 | 65/65 | 0.90 | 0.18 | 189,202,210,216             | 0     |
| 22  | CLA  | B     | 1023 | 65/65 | 0.91 | 0.11 | 174,179,181,191             | 0     |
| 22  | CLA  | c     | 6030 | 65/65 | 0.91 | 0.10 | 185,197,216,216             | 0     |
| 22  | CLA  | B     | 1012 | 65/65 | 0.91 | 0.11 | 160,167,172,174             | 0     |
| 22  | CLA  | A     | 1007 | 65/65 | 0.91 | 0.14 | 129,174,204,205             | 0     |
| 22  | CLA  | B     | 1022 | 65/65 | 0.91 | 0.11 | 138,180,198,200             | 0     |
| 22  | CLA  | A     | 1003 | 65/65 | 0.92 | 0.14 | 160,169,175,212             | 0     |
| 22  | CLA  | C     | 1031 | 65/65 | 0.92 | 0.14 | 181,185,202,216             | 0     |
| 22  | CLA  | B     | 1015 | 65/65 | 0.92 | 0.12 | 177,182,185,216             | 0     |
| 22  | CLA  | c     | 6033 | 65/65 | 0.92 | 0.14 | 138,185,199,200             | 0     |
| 22  | CLA  | C     | 1033 | 65/65 | 0.92 | 0.16 | 138,185,199,200             | 0     |
| 22  | CLA  | H     | 1017 | 65/65 | 0.92 | 0.15 | 169,197,201,208             | 0     |
| 27  | IOD  | t     | 6066 | 1/1   | 0.92 | 0.08 | 199,199,199,199             | 0     |
| 22  | CLA  | B     | 1010 | 65/65 | 0.92 | 0.15 | 160,183,186,189             | 0     |
| 22  | CLA  | b     | 6018 | 65/65 | 0.93 | 0.14 | 172,186,191,192             | 0     |
| 22  | CLA  | b     | 6010 | 65/65 | 0.93 | 0.12 | 160,183,186,189             | 0     |
| 22  | CLA  | b     | 6020 | 65/65 | 0.93 | 0.15 | 167,175,180,197             | 0     |
| 22  | CLA  | D     | 1004 | 65/65 | 0.93 | 0.15 | 130,168,179,181             | 0     |
| 22  | CLA  | B     | 1016 | 65/65 | 0.93 | 0.12 | 130,172,175,180             | 0     |
| 30  | FE2  | a     | 6002 | 1/1   | 0.93 | 0.14 | 148,148,148,148             | 0     |
| 31  | HEM  | F     | 1040 | 43/43 | 0.93 | 0.17 | 186,215,216,216             | 0     |
| 22  | CLA  | b     | 6023 | 65/65 | 0.93 | 0.11 | 174,179,181,191             | 0     |
| 22  | CLA  | b     | 6013 | 65/65 | 0.94 | 0.17 | 146,173,183,184             | 0     |
| 22  | CLA  | B     | 1018 | 65/65 | 0.94 | 0.13 | 172,186,191,192             | 0     |
| 31  | HEM  | V     | 1041 | 43/43 | 0.94 | 0.23 | 131,181,185,187             | 0     |
| 22  | CLA  | B     | 1013 | 65/65 | 0.94 | 0.14 | 146,173,183,184             | 0     |
| 31  | HEM  | v     | 6041 | 43/43 | 0.94 | 0.15 | 131,181,185,187             | 0     |
| 30  | FE2  | D     | 1002 | 1/1   | 0.95 | 0.09 | 148,148,148,148             | 0     |
| 22  | CLA  | d     | 6004 | 65/65 | 0.95 | 0.13 | 130,168,179,181             | 0     |
| 27  | IOD  | a     | 6065 | 1/1   | 0.96 | 0.06 | 158,158,158,158             | 0     |
| 22  | CLA  | B     | 1020 | 65/65 | 0.96 | 0.13 | 167,175,180,197             | 0     |
| 21  | OEC  | a     | 6001 | 5/9   | 0.98 | 0.09 | 132,148,162,172             | 0     |
| 27  | IOD  | A     | 1065 | 1/1   | 0.98 | 0.04 | 158,158,158,158             | 0     |
| 21  | OEC  | A     | 1001 | 5/9   | 0.98 | 0.07 | 132,148,162,172             | 0     |
| 27  | IOD  | D     | 1064 | 1/1   | 0.98 | 0.03 | 160,160,160,160             | 0     |
| 27  | IOD  | d     | 6064 | 1/1   | 0.99 | 0.04 | 160,160,160,160             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

**Electron density around CLA K 1034:**

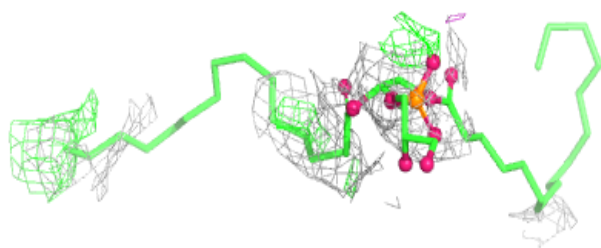
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





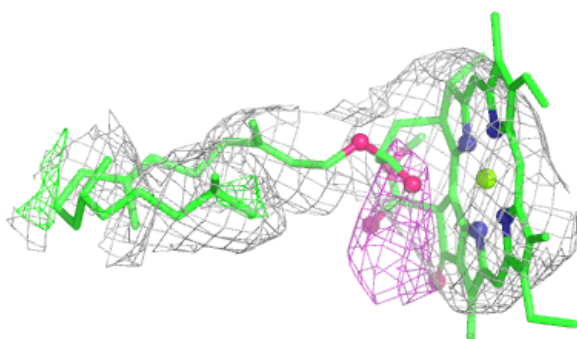
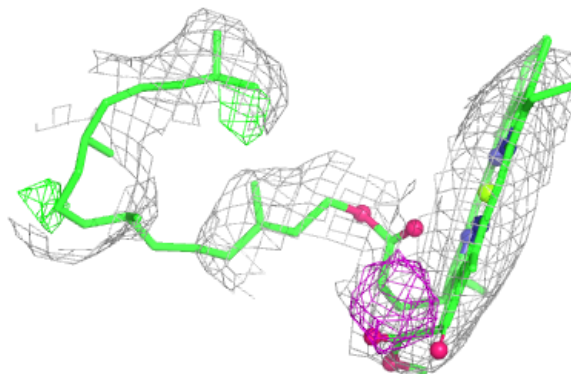
**Electron density around LHG a 6063:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



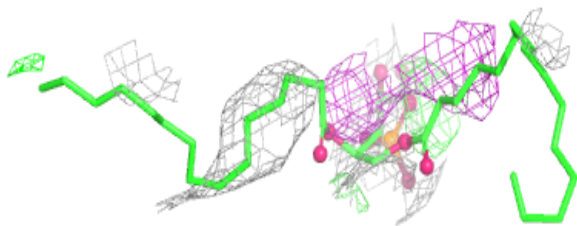
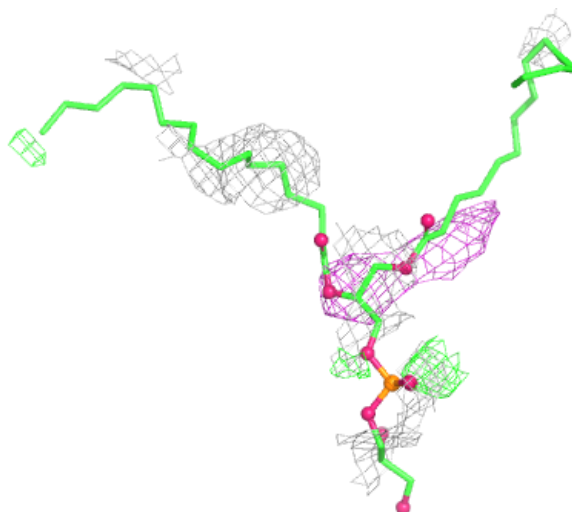
**Electron density around CLA B 1009:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



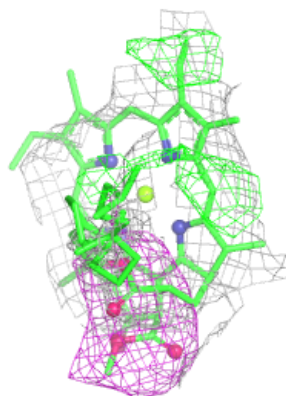
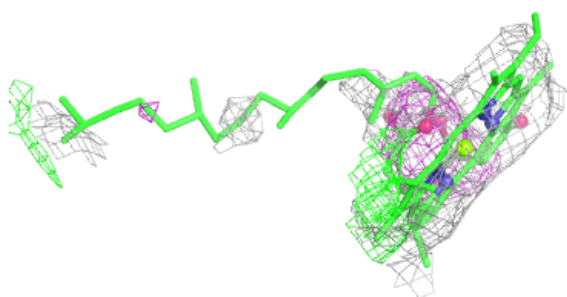
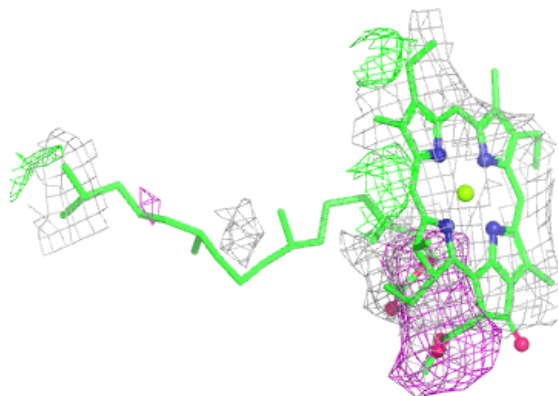
**Electron density around LHG A 1063:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

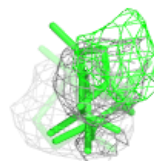
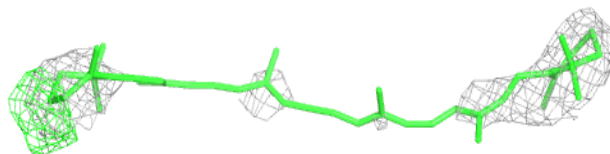
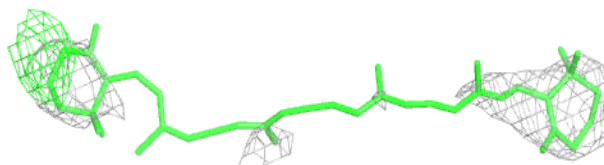


**Electron density around CLA k 6034:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

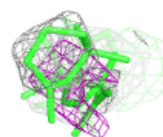
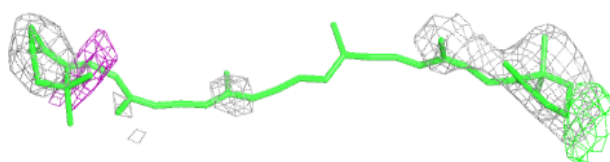
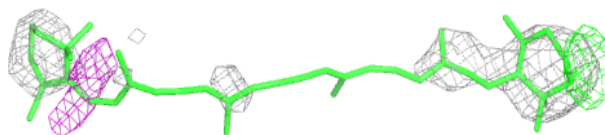
**Electron density around BCR T 6048:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

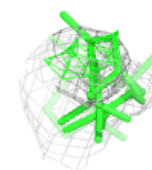
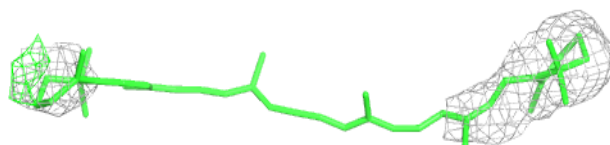
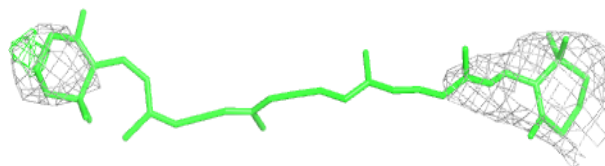


**Electron density around BCR A 1044:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

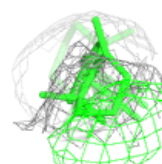
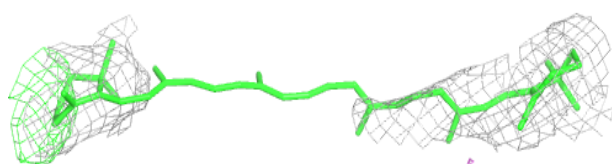
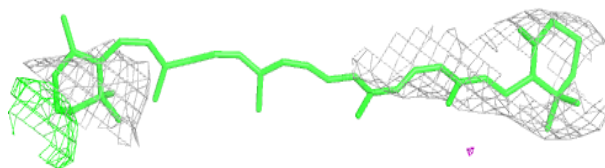
**Electron density around BCR B 1048:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

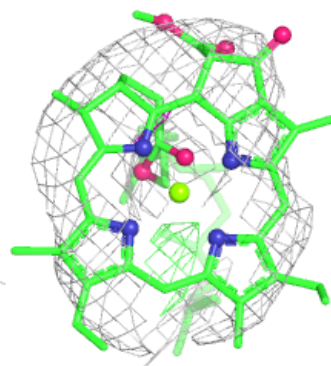
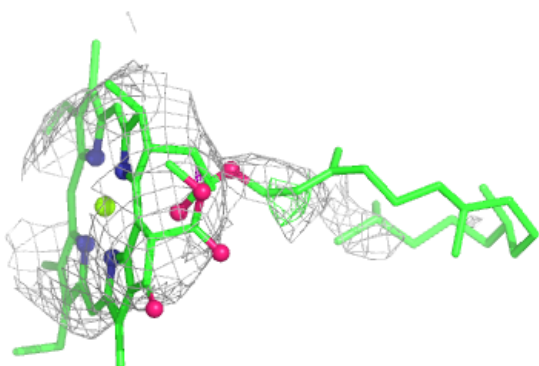
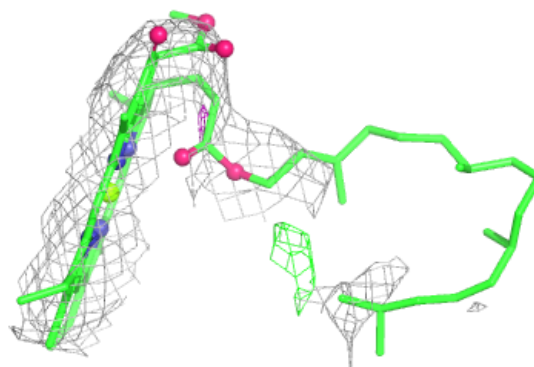


**Electron density around BCR b 6047:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

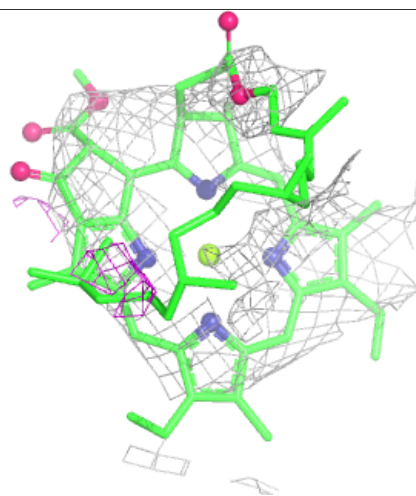
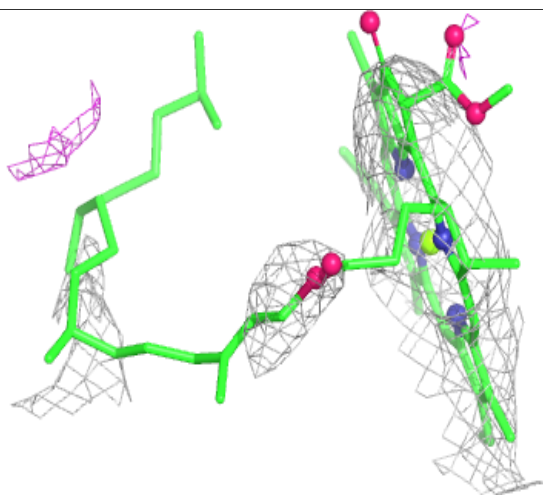
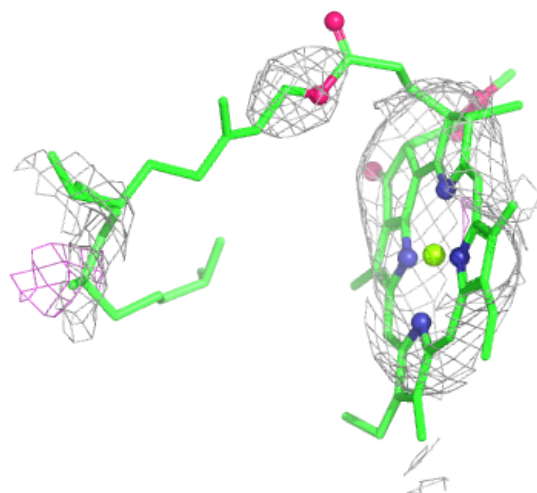
**Electron density around CLA b 6009:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 6037:**

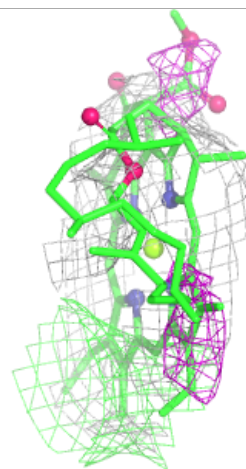
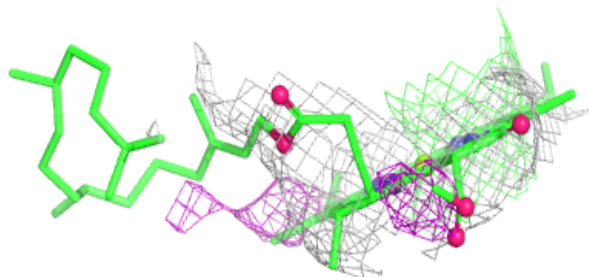
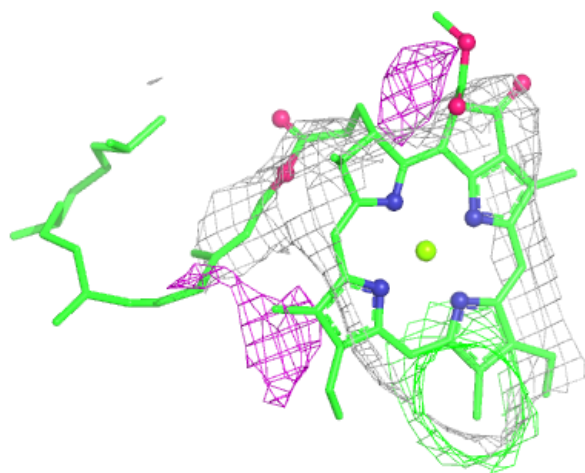
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





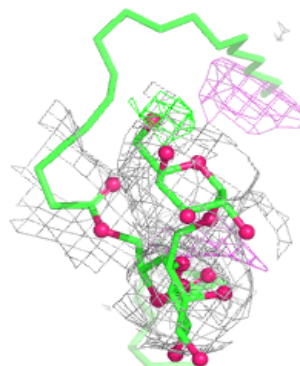
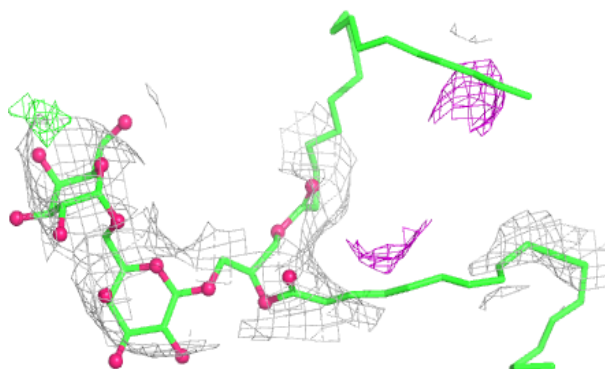
**Electron density around CLA c 6027:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

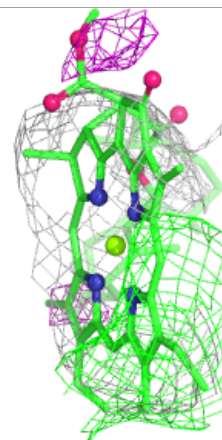
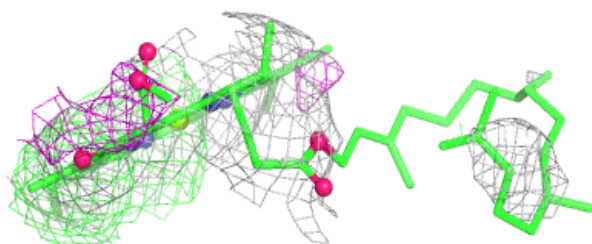
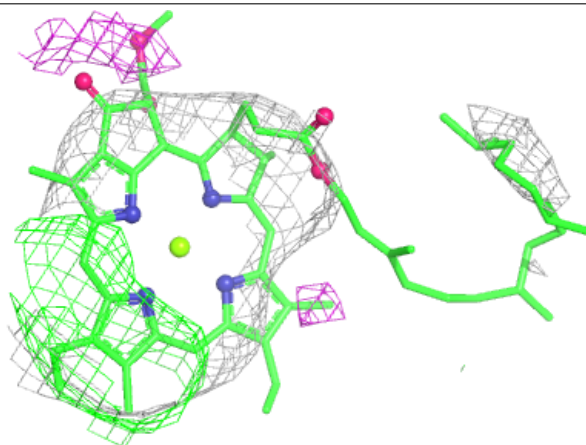


**Electron density around DGD C 1056:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

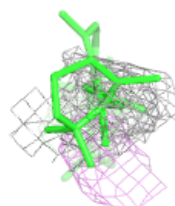
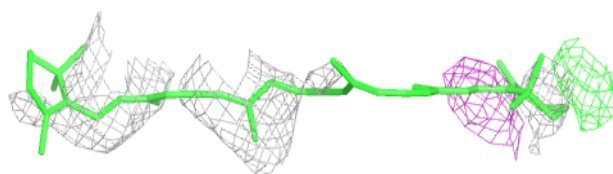
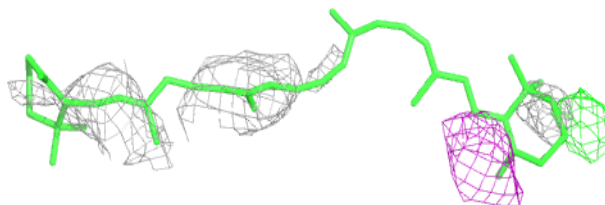
**Electron density around CLA C 1027:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

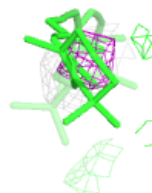
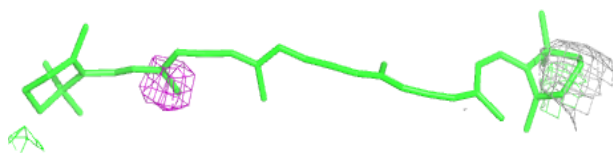
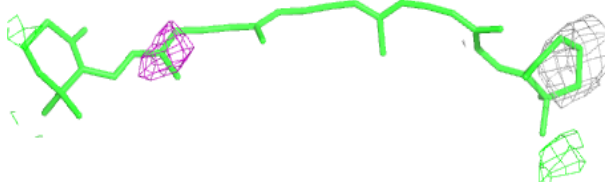


**Electron density around BCR c 6054:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

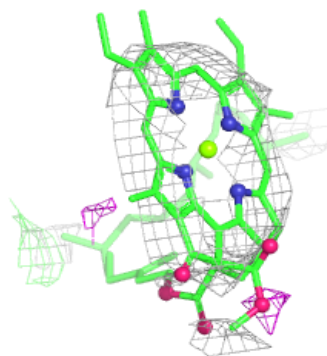
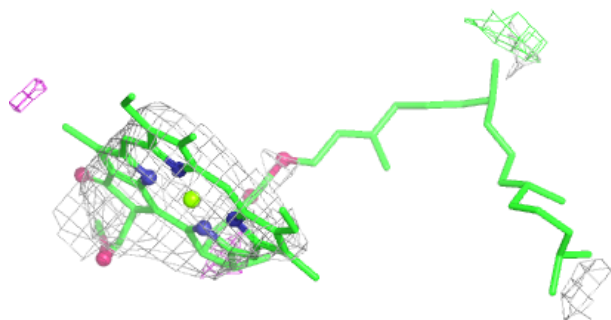
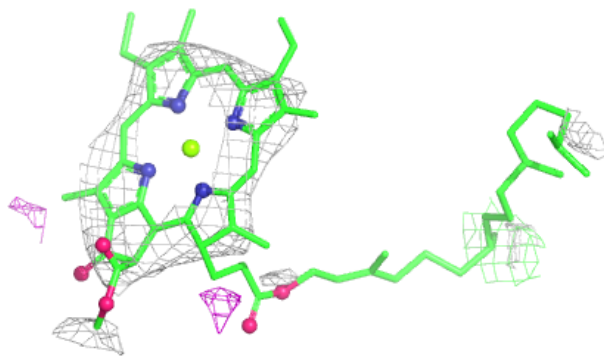
**Electron density around BCR k 6052:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

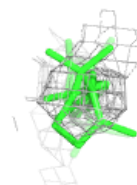
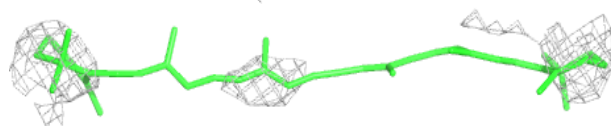
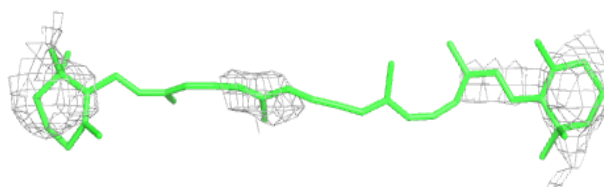


**Electron density around CLA d 6008:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

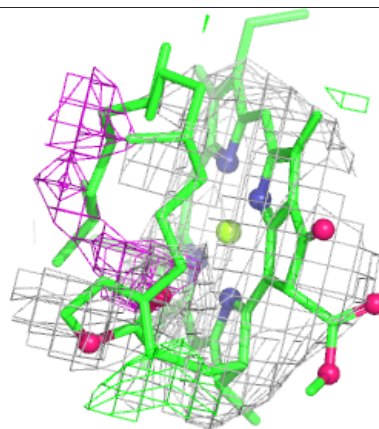
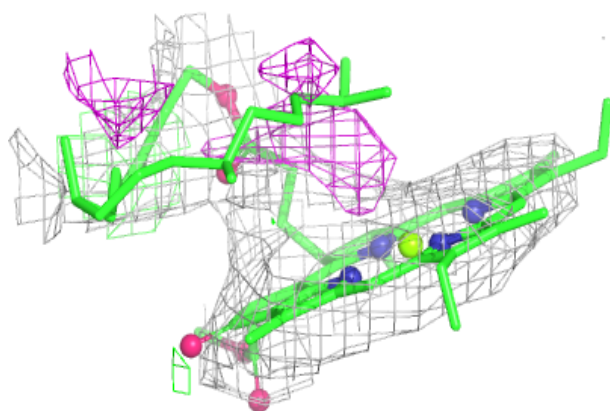
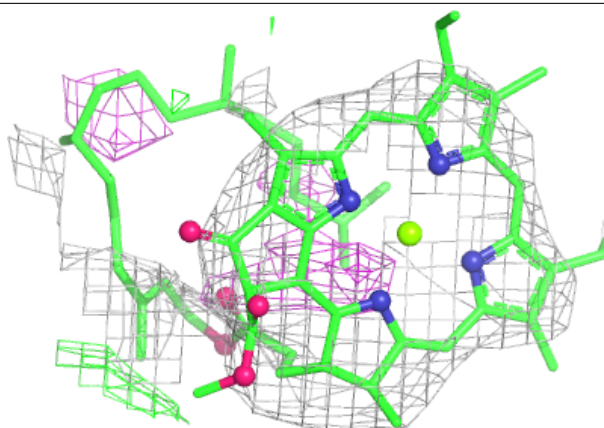
**Electron density around BCR Z 1053:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

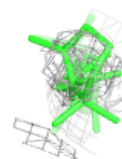
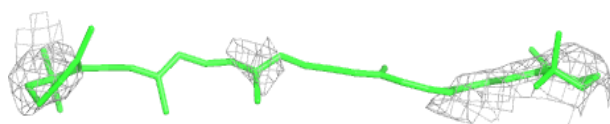
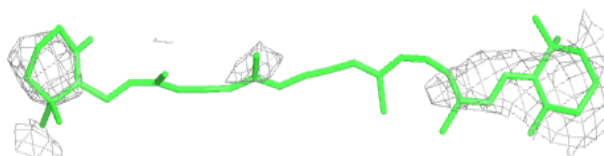


**Electron density around CLA c 6026:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

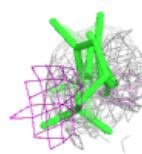
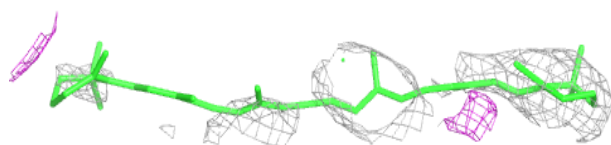
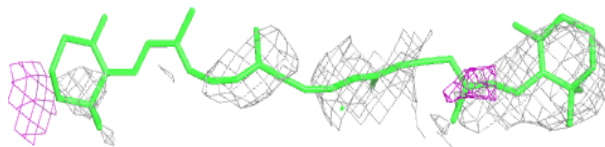
**Electron density around BCR z 6053:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

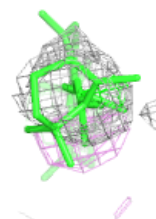
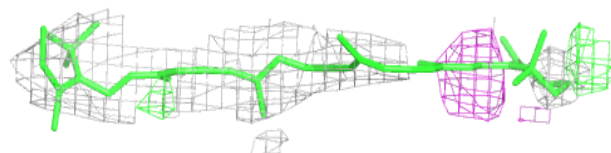


**Electron density around BCR b 6045:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR C 1054:**

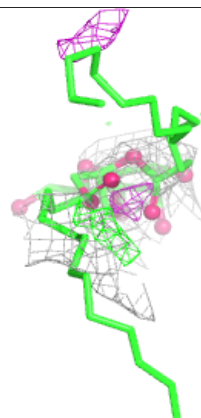
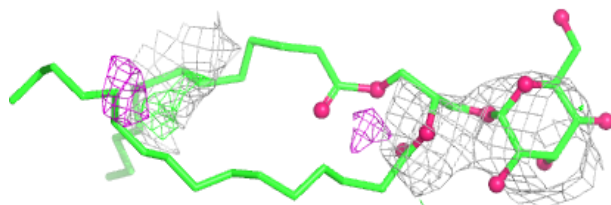
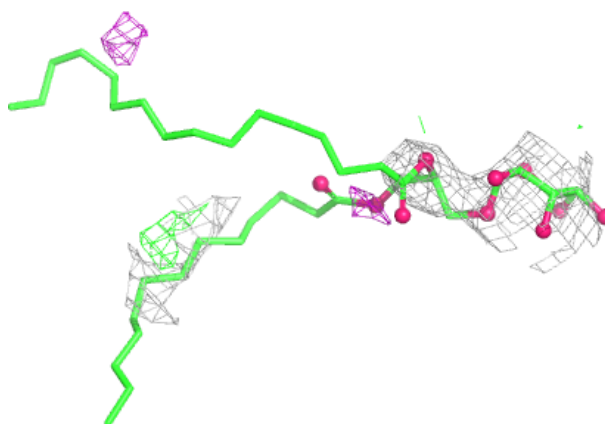
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



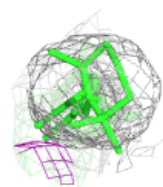
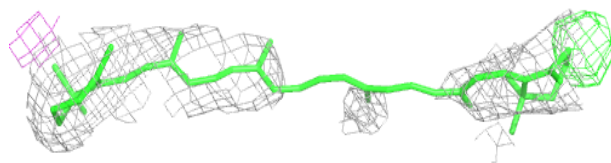
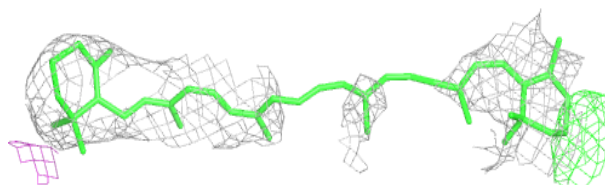


**Electron density around MGE d 6062:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR B 1047:**

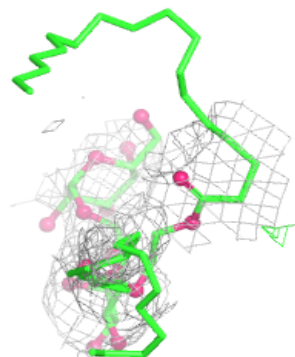
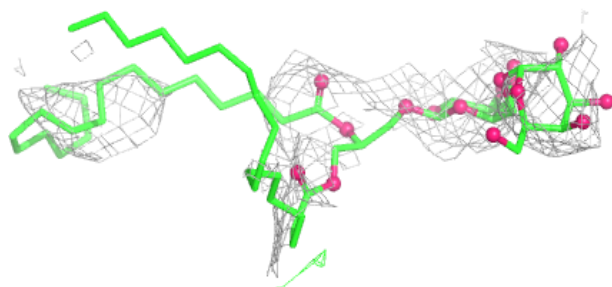
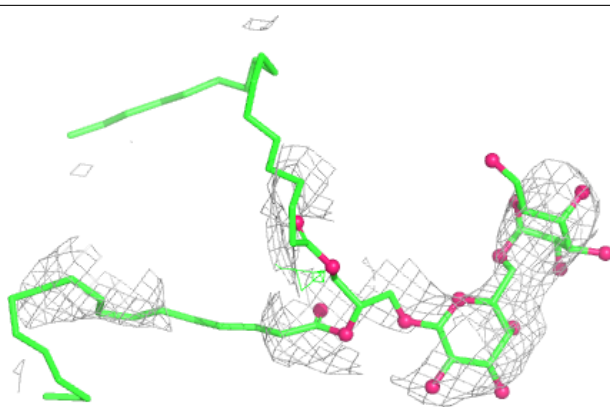
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



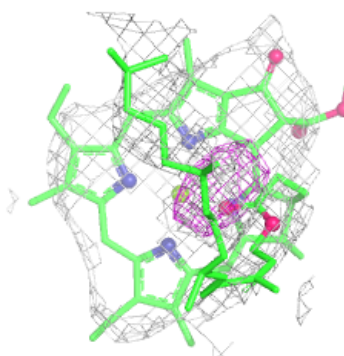
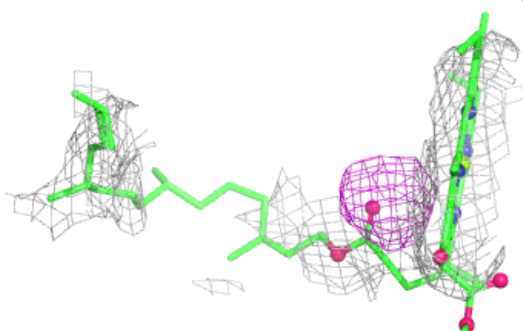
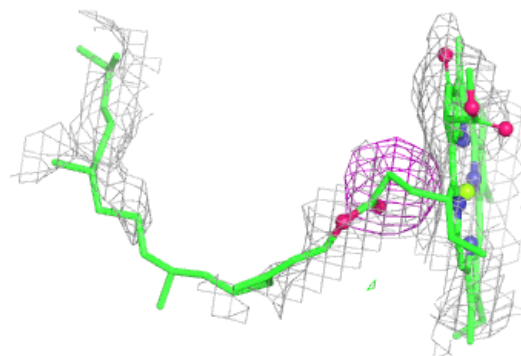


**Electron density around DGD c 6056:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

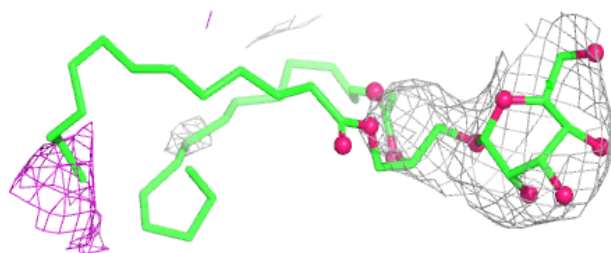
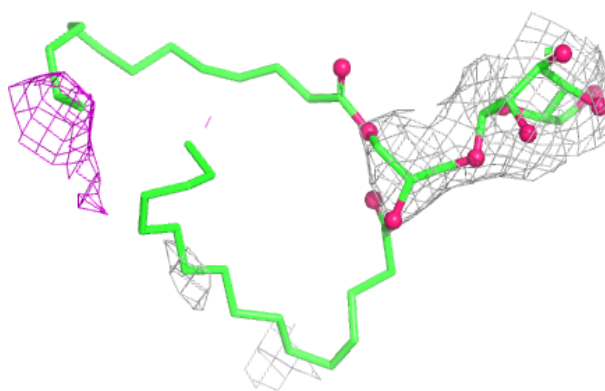
**Electron density around CLA b 6014:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

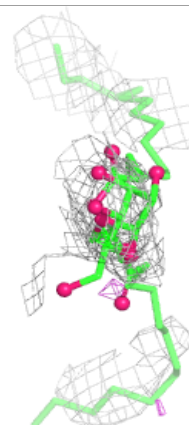
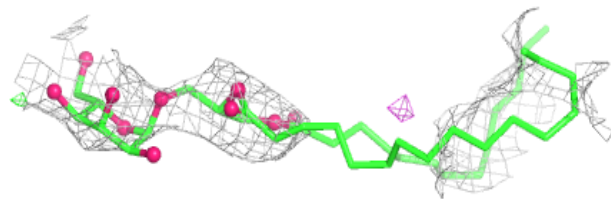
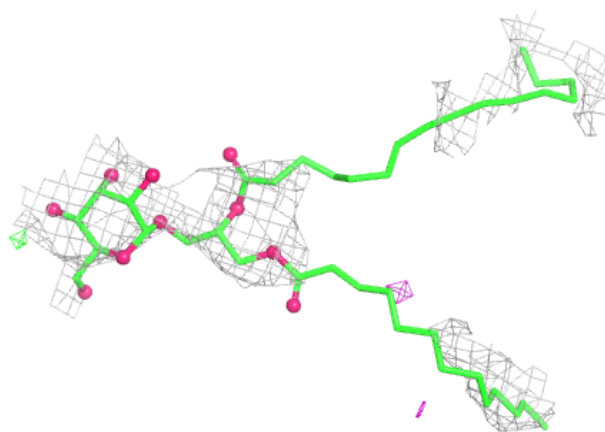


**Electron density around MGE B 1060:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

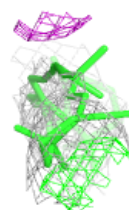
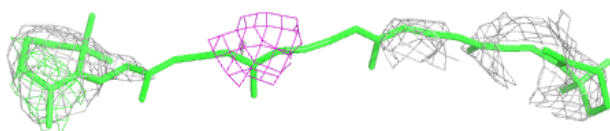
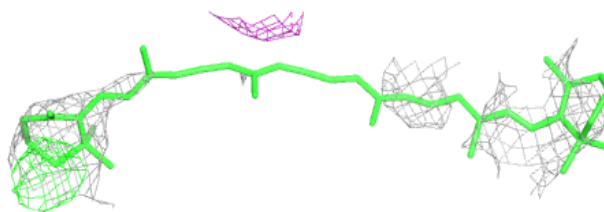
**Electron density around MGE D 1059:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



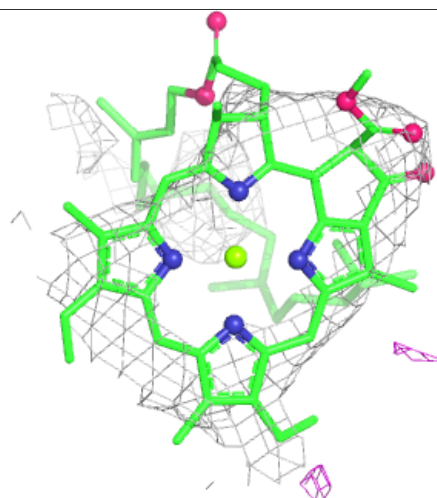
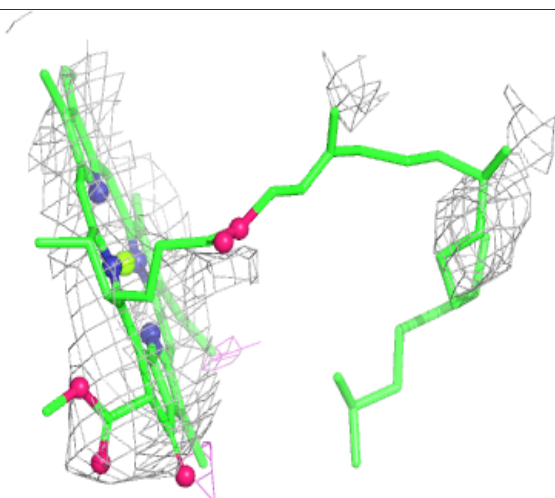
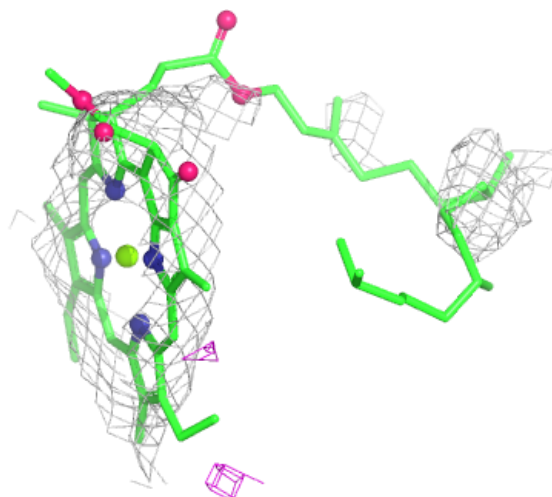
**Electron density around BCR T 6046:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



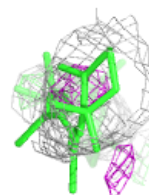
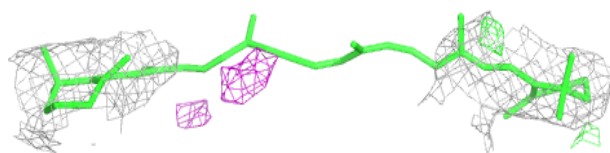
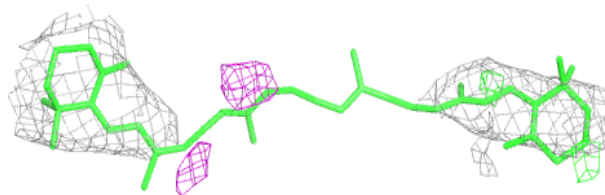
**Electron density around CLA C 1037:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

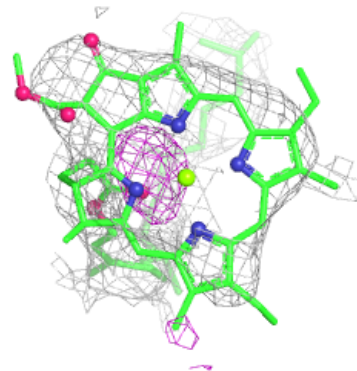
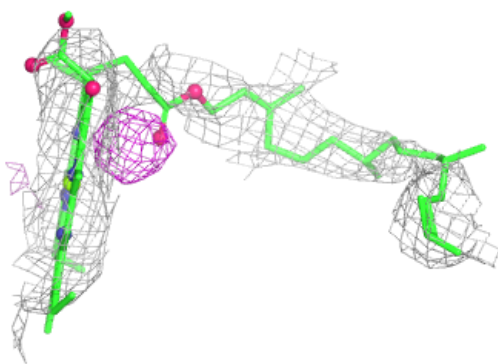
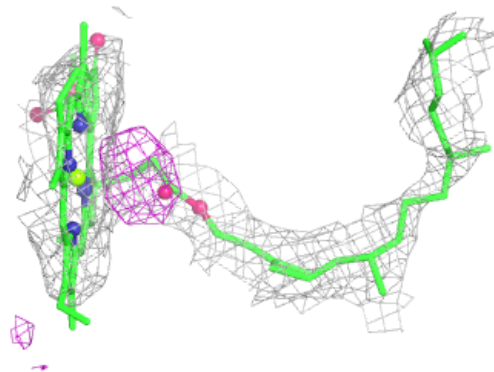


**Electron density around BCR d 6050:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

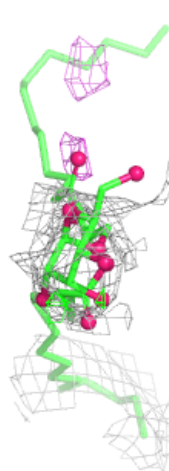
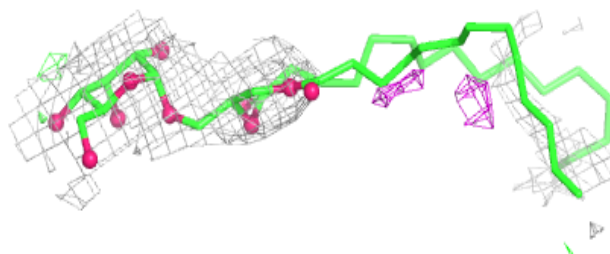
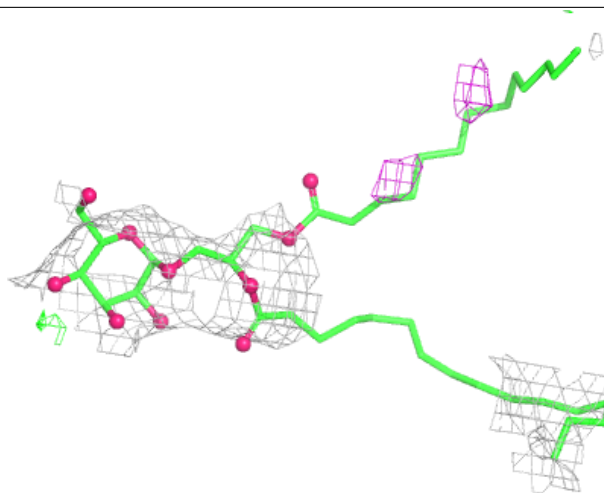
**Electron density around CLA B 1014:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



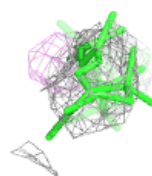
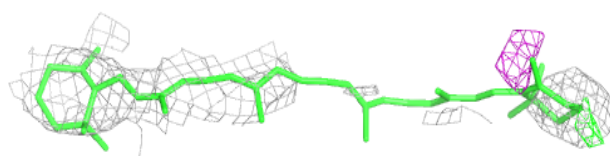
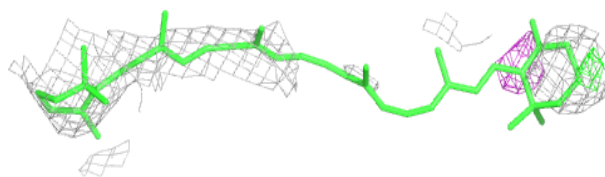
**Electron density around MGE d 6059:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

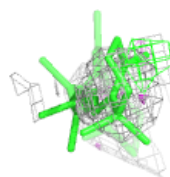
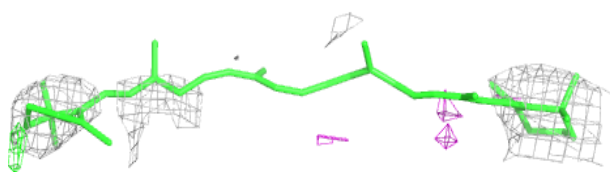
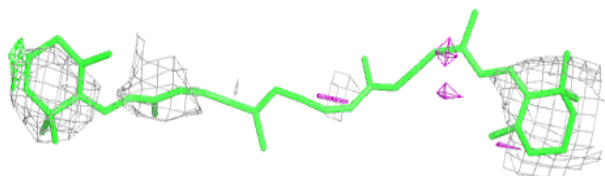


**Electron density around BCR h 6049:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR D 1050:**

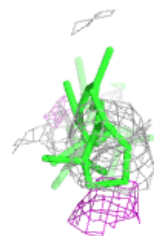
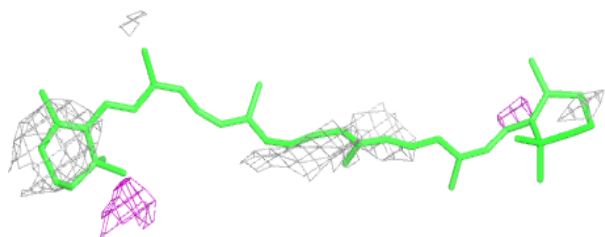
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



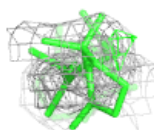
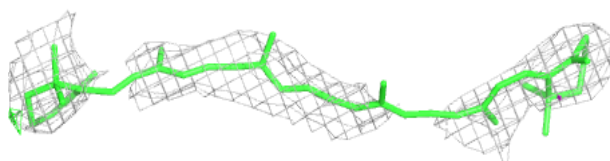
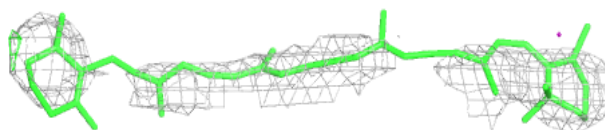


**Electron density around BCR K 1051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

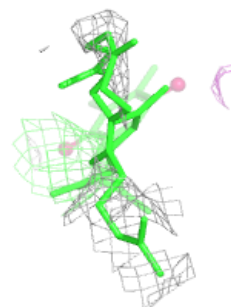
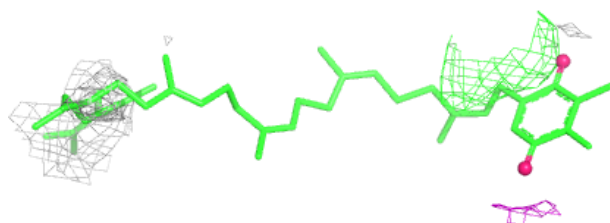
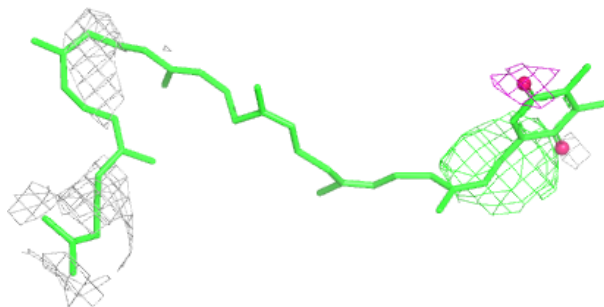
**Electron density around BCR a 6044:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



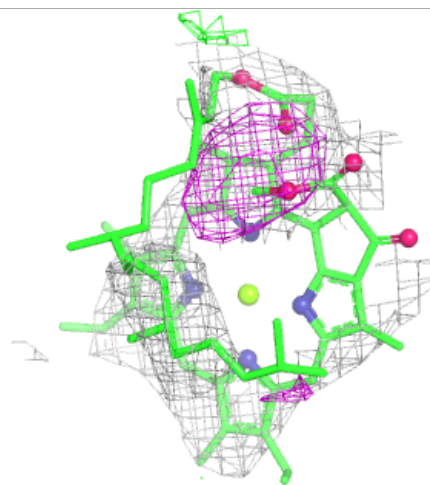
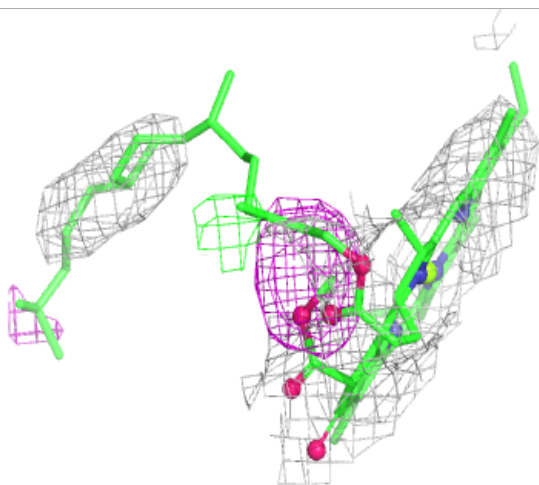
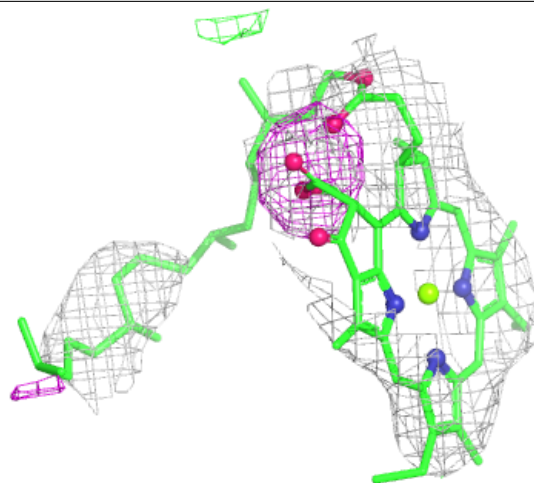
**Electron density around PQ9 A 1043:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



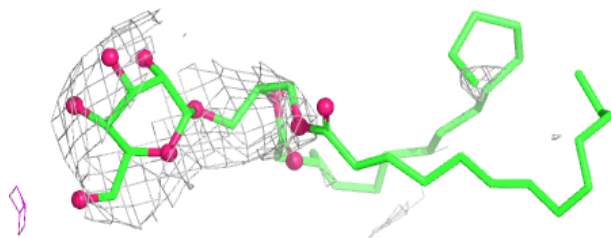
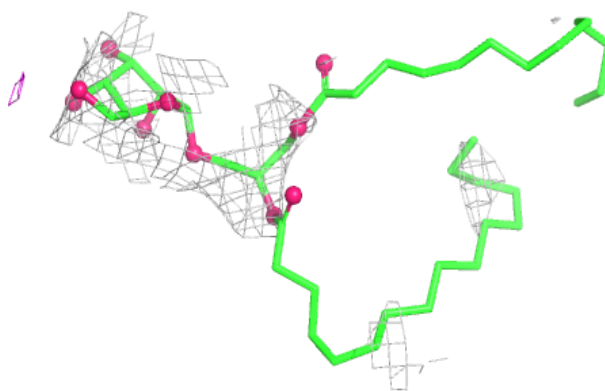
**Electron density around CLA b 6021:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

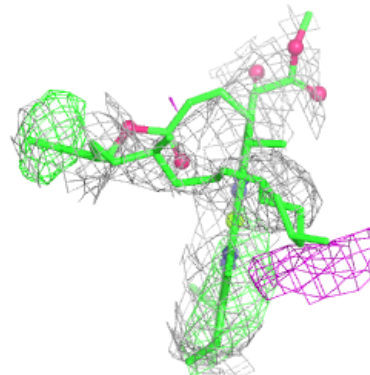
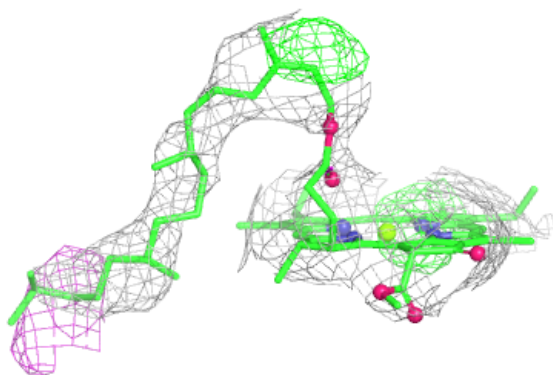
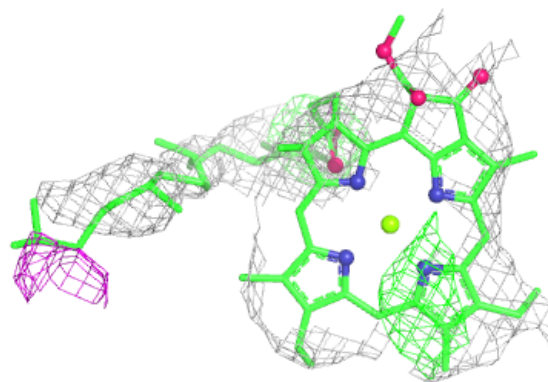


**Electron density around MGE b 6060:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

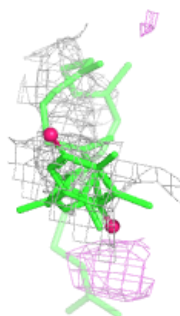
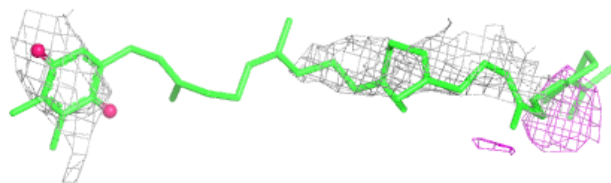
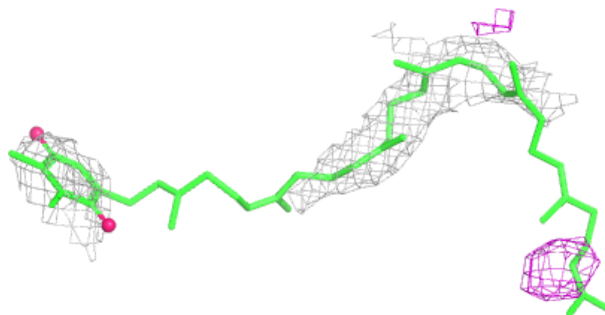
**Electron density around CLA d 6005:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



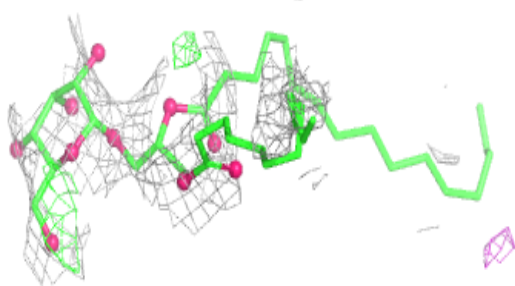
**Electron density around PQ9 d 6042:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



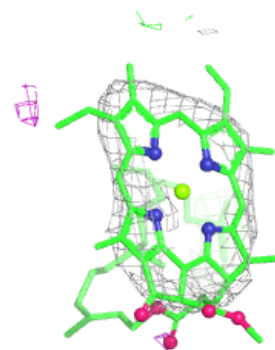
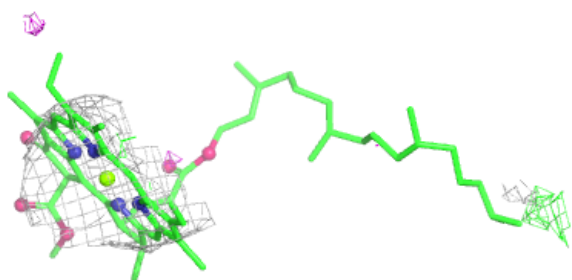
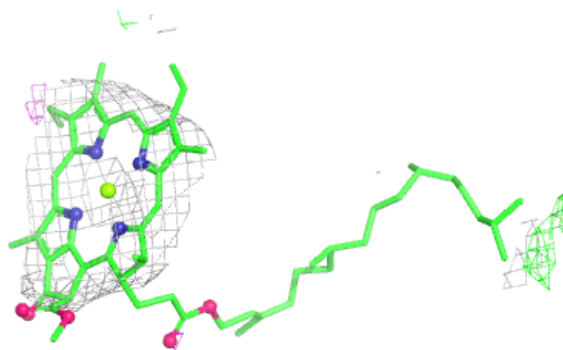
**Electron density around MGE 1 6061:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

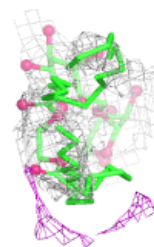
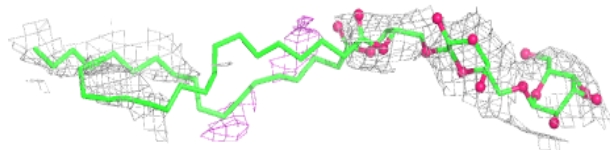


**Electron density around CLA c 6035:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DGD C 1057:**

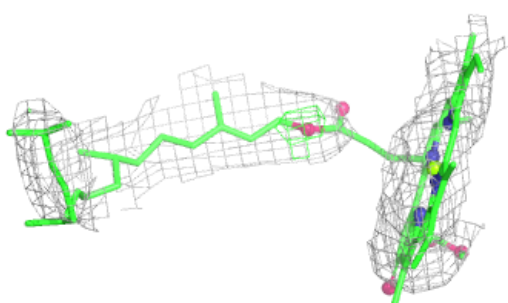
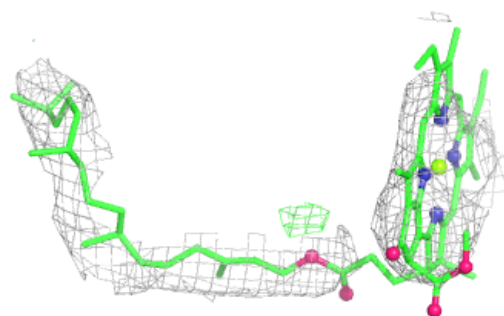
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



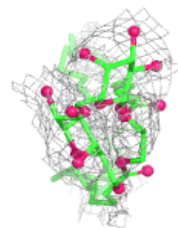
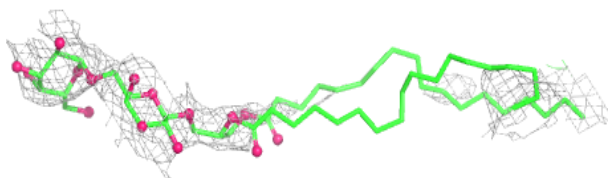
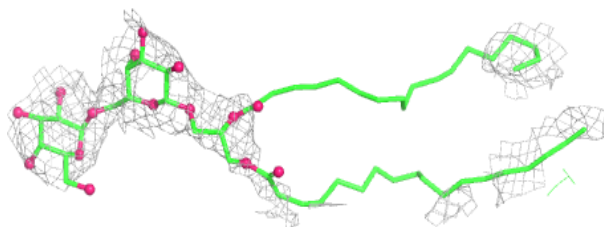


**Electron density around CLA C 1030:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

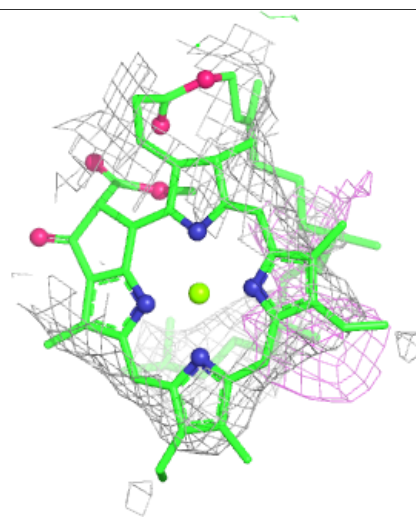
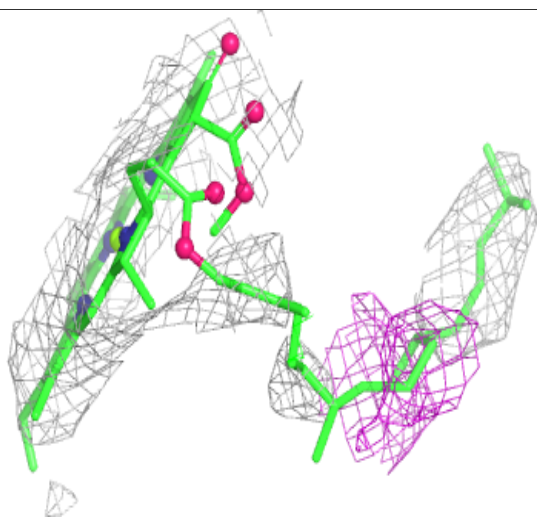
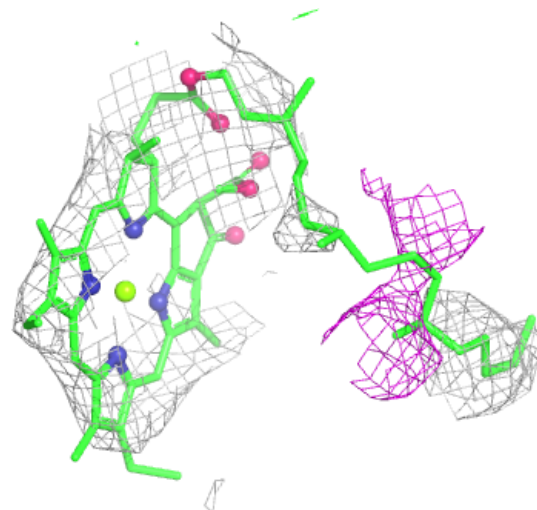
**Electron density around DGD c 6057:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



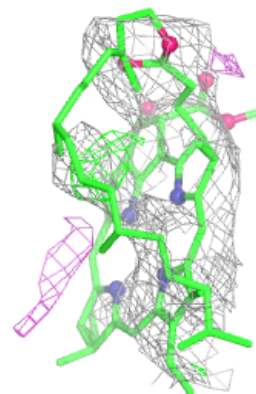
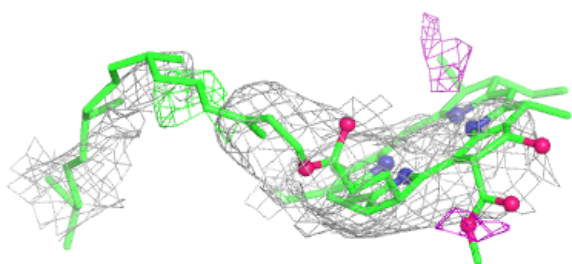
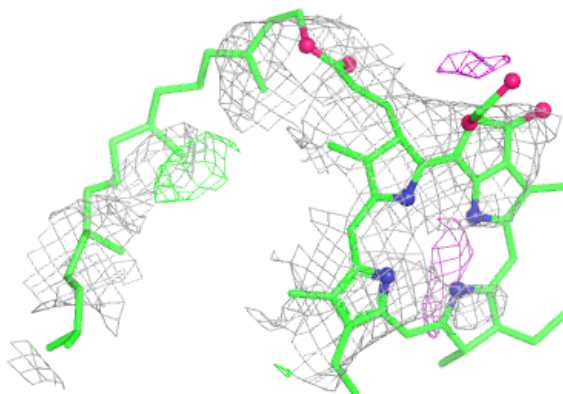
**Electron density around CLA B 1021:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

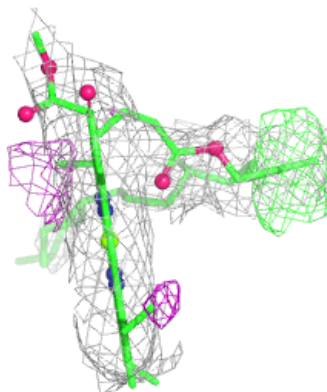
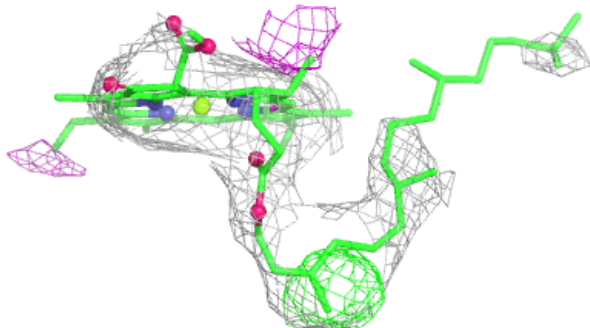
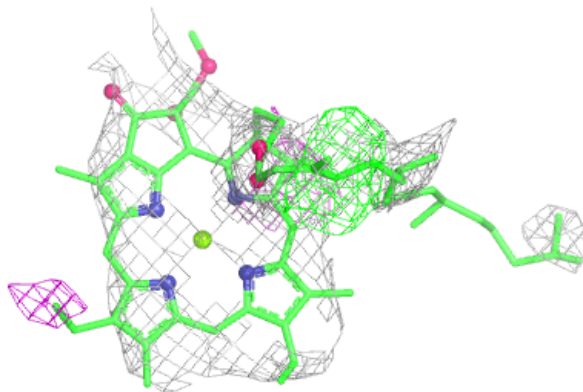


**Electron density around PHO D 1039:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

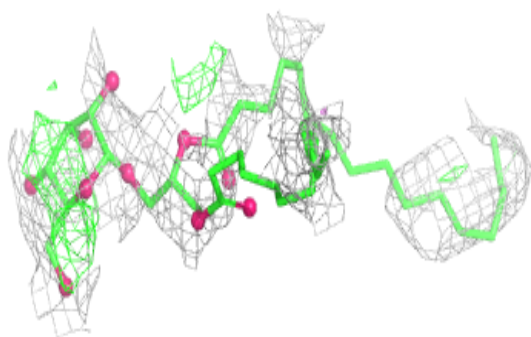
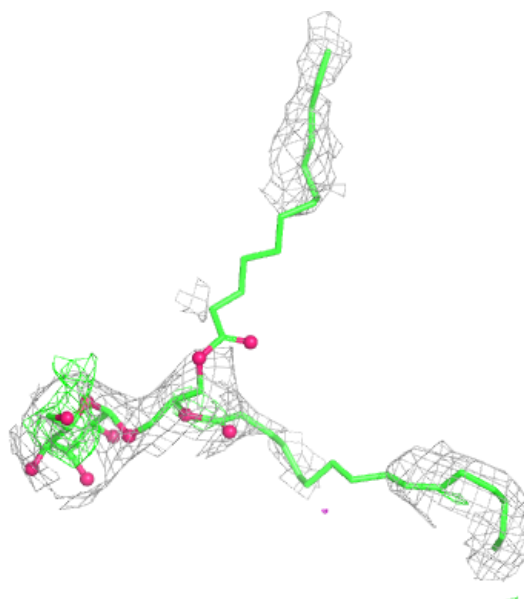
**Electron density around CLA D 1005:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



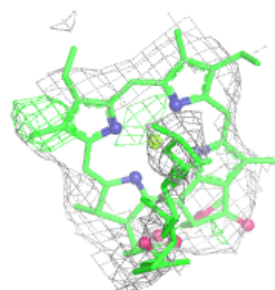
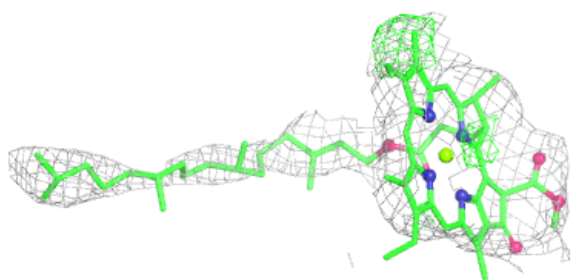
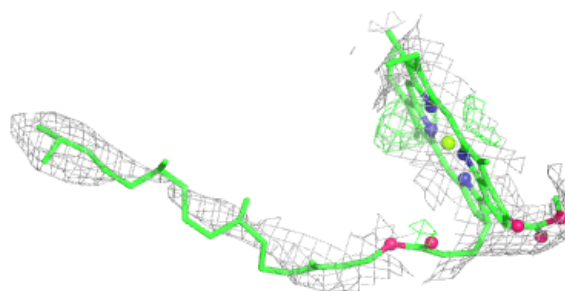
**Electron density around MGE L 1061:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

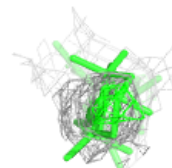
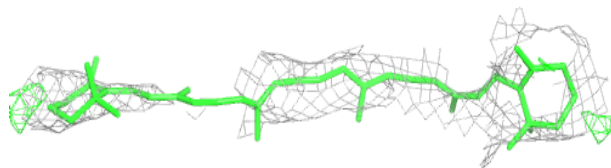
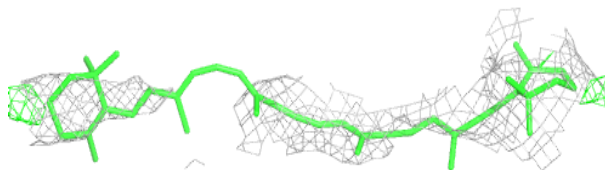


**Electron density around CLA b 6015:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

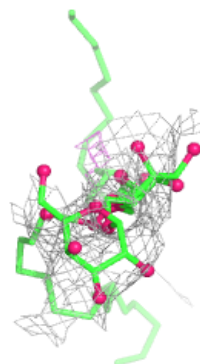
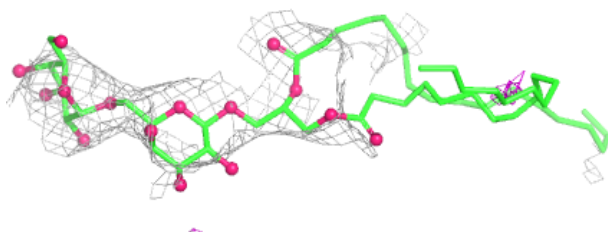
**Electron density around BCR H 1049:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

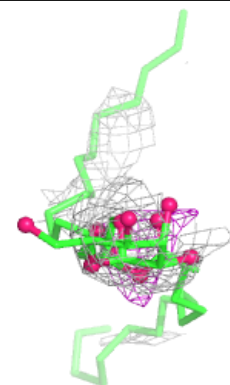
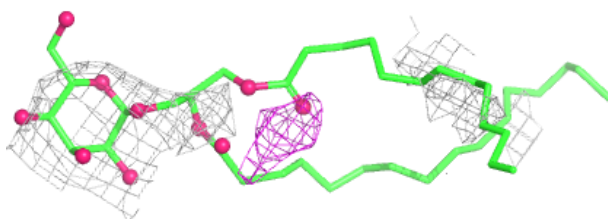
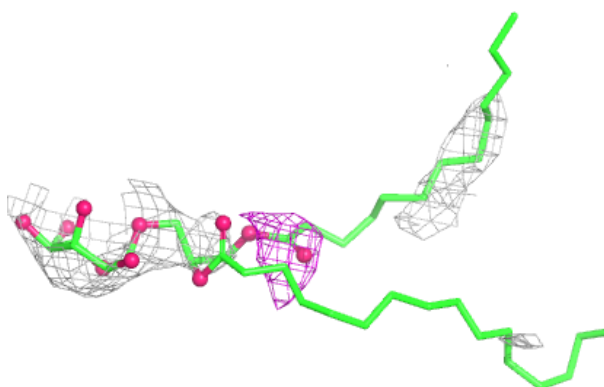


**Electron density around DGD c 6055:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MGE D 1062:**

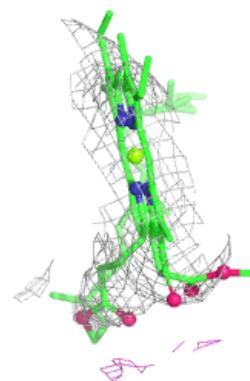
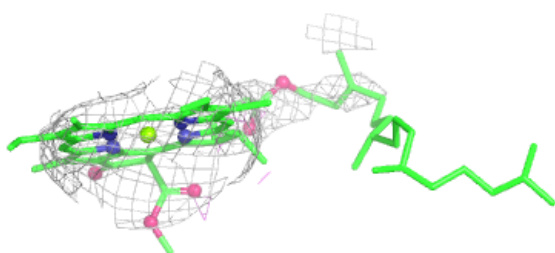
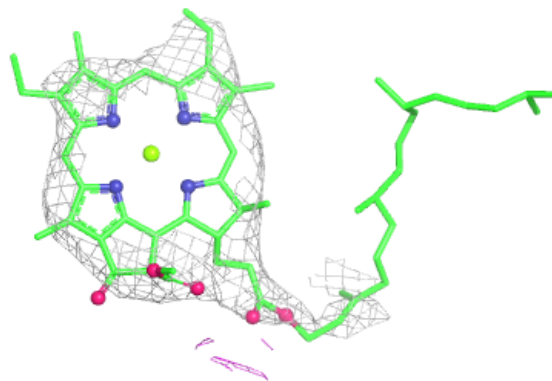
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



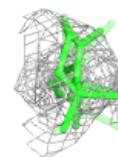
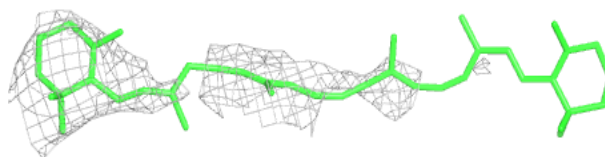


**Electron density around CLA C 1036:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR B 1045:**

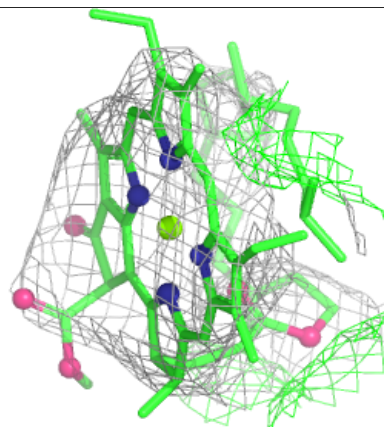
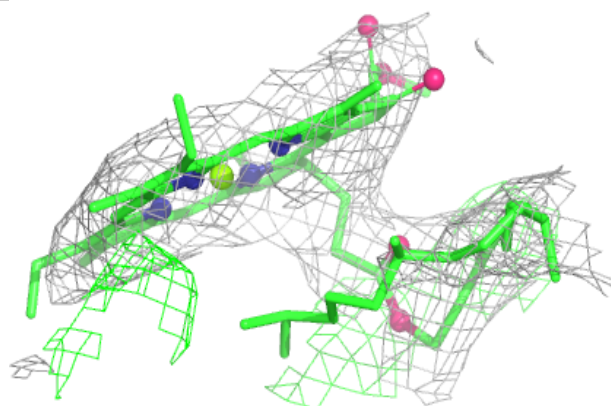
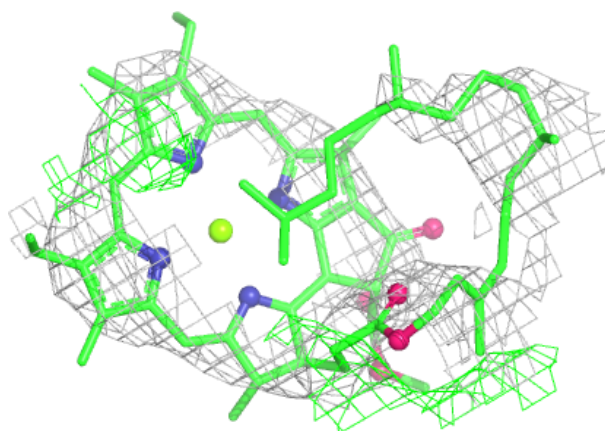
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



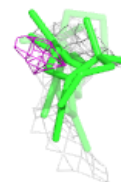
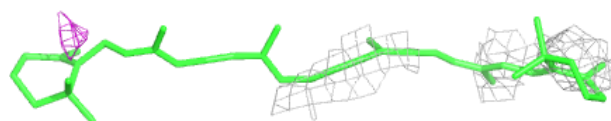
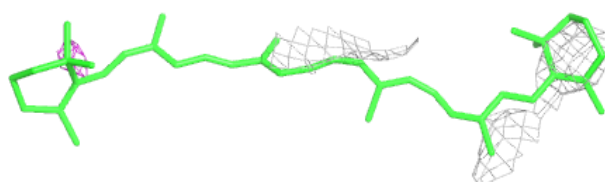


**Electron density around CLA C 1026:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

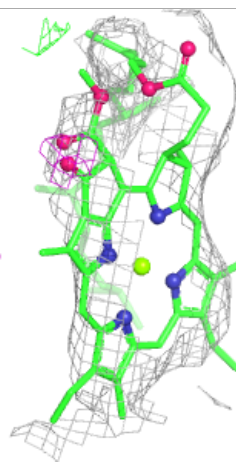
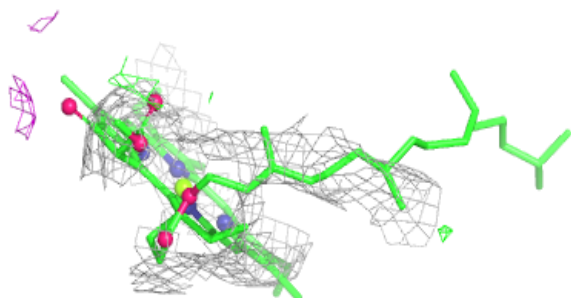
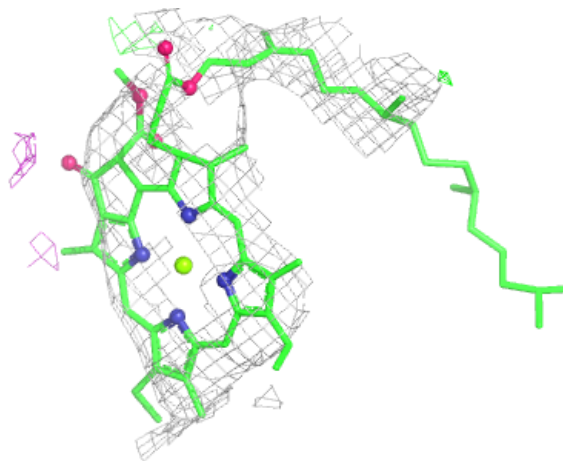
**Electron density around BCR k 6051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



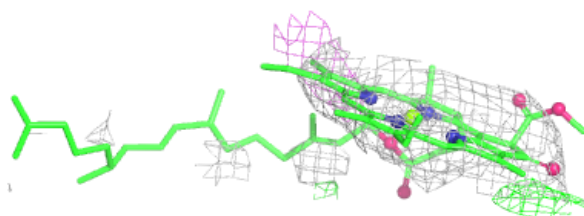
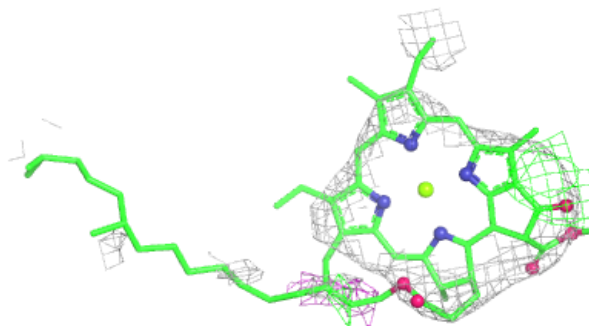
**Electron density around CLA b 6024:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

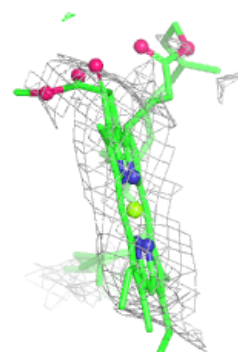
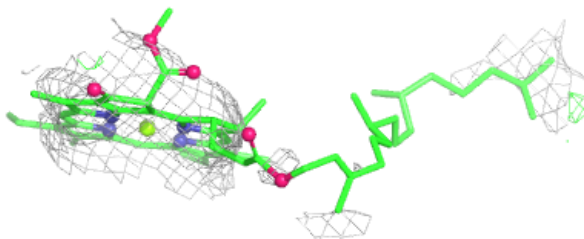
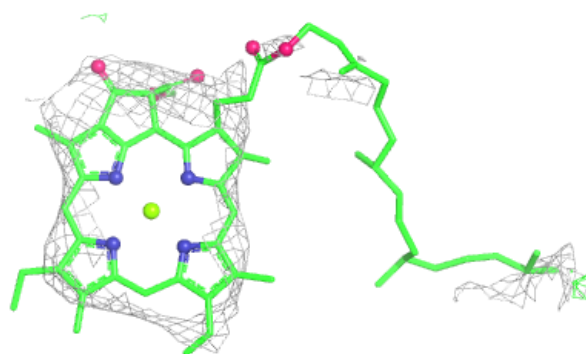


**Electron density around CLA c 6025:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

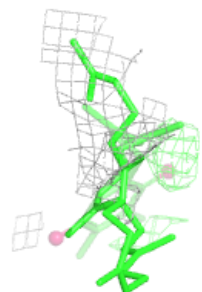
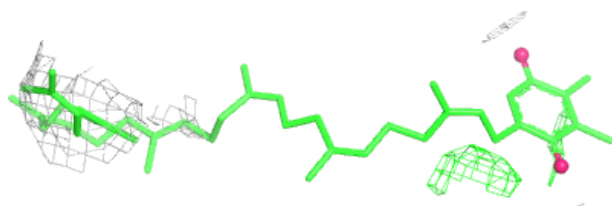
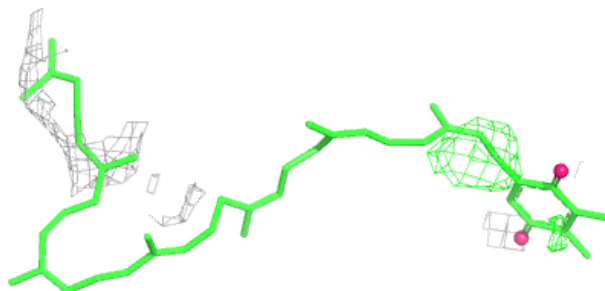
**Electron density around CLA c 6036:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

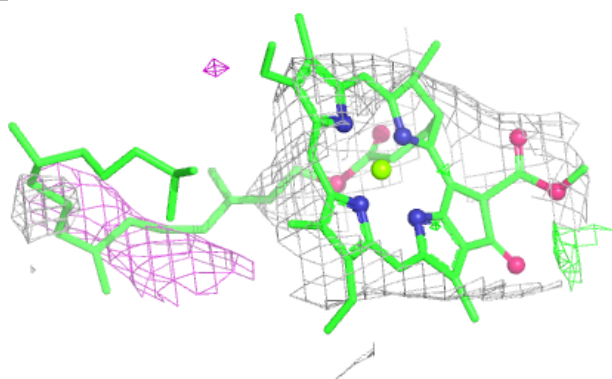
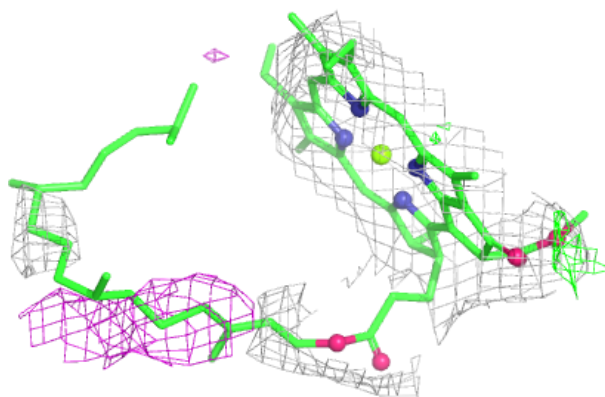


**Electron density around PQ9 a 6043:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

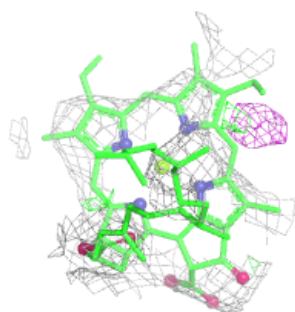
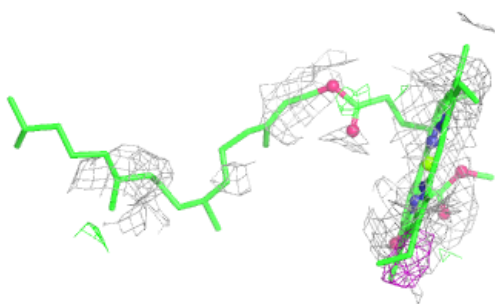
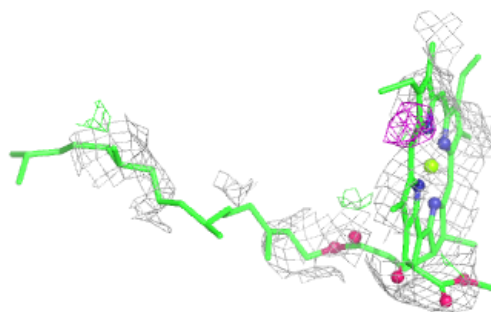
**Electron density around CLA C 1028:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



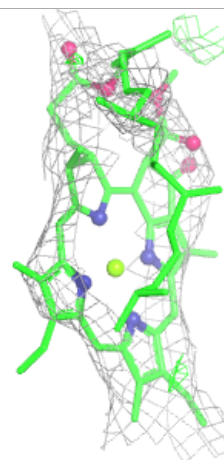
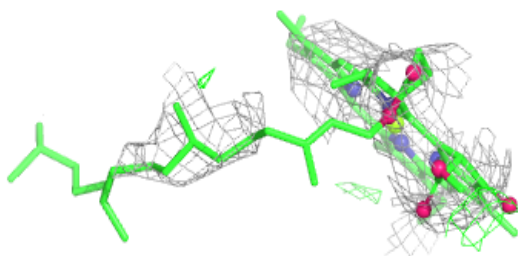
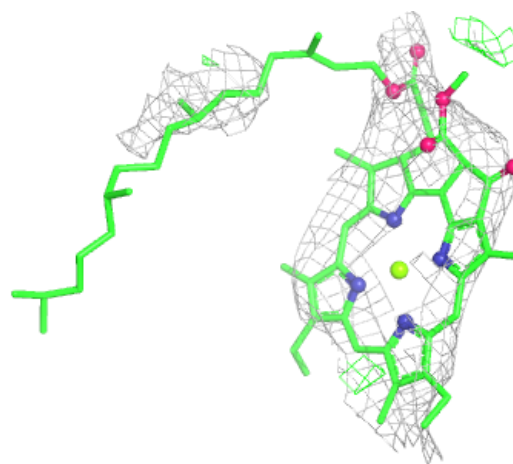
**Electron density around CLA c 6032:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1024:**

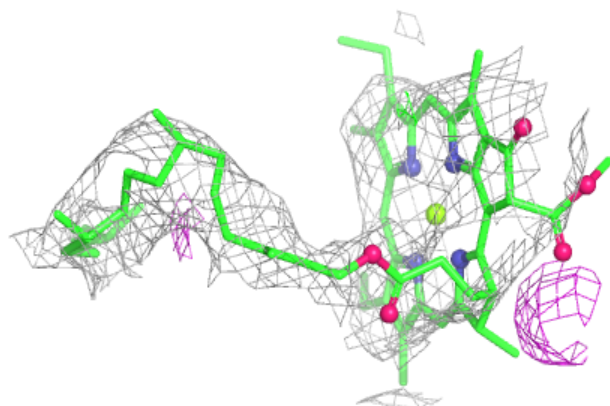
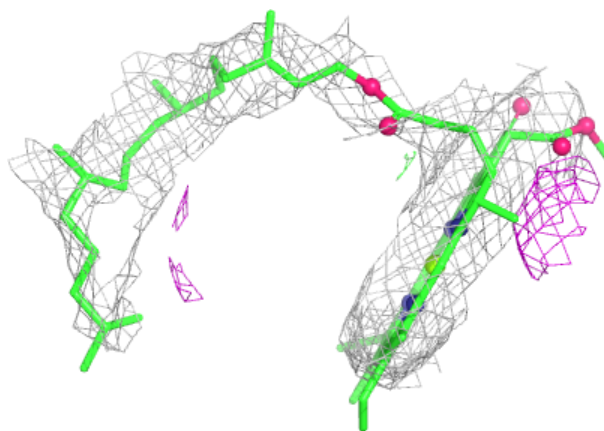
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



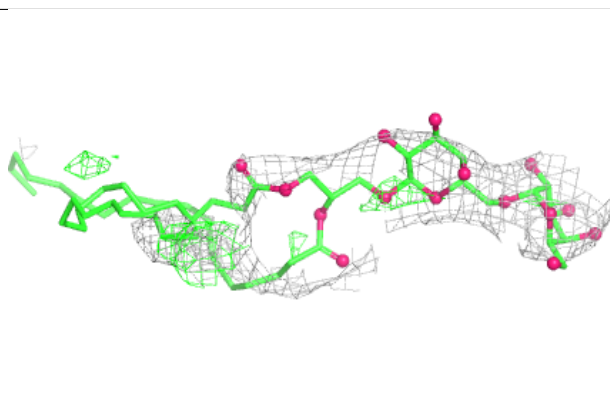
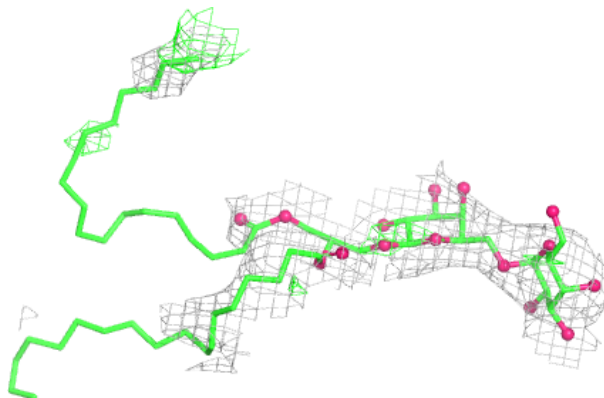


**Electron density around CLA b 6019:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DGD C 1055:**

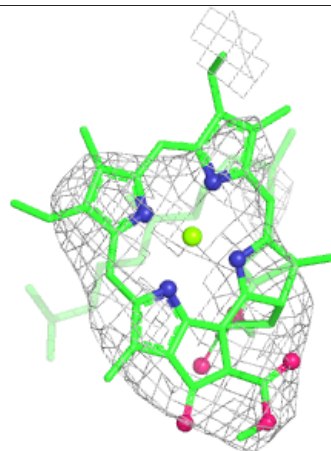
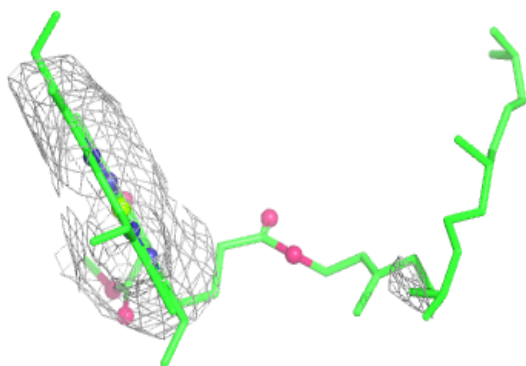
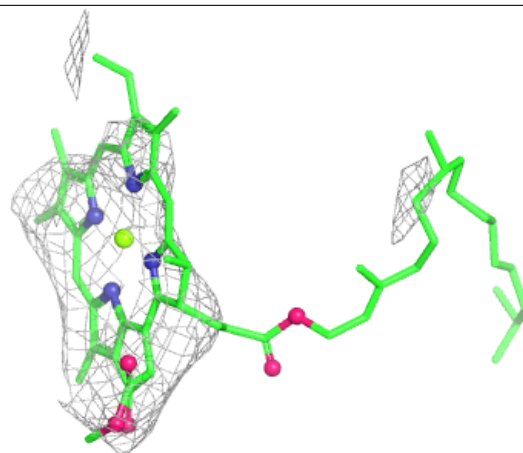
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



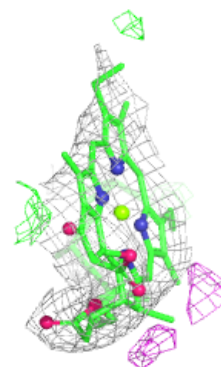
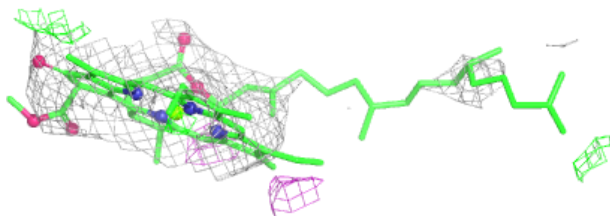
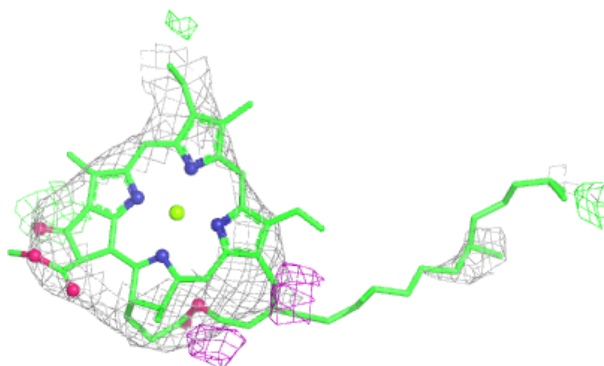


**Electron density around CLA a 6007:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

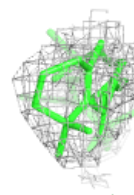
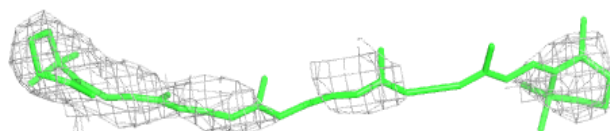
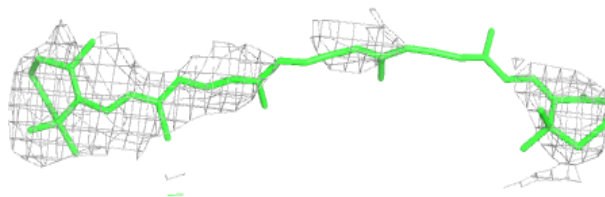
**Electron density around CLA C 1025:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

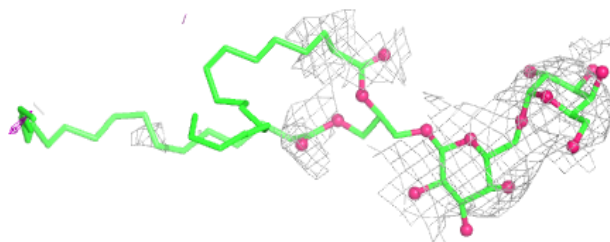


**Electron density around BCR t 1046:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

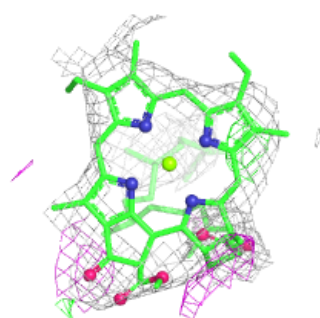
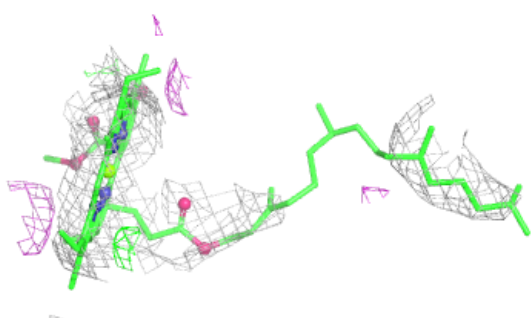
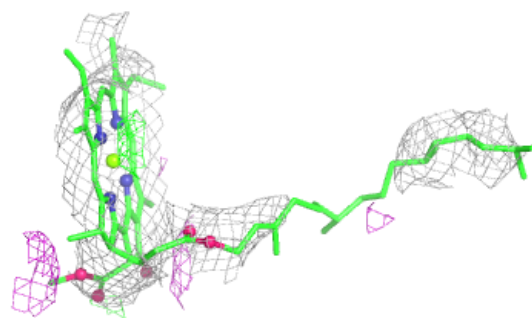
**Electron density around DGD B 1058:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

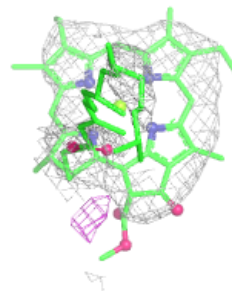
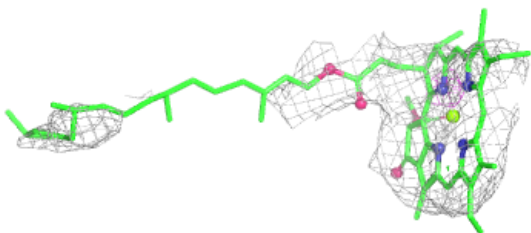
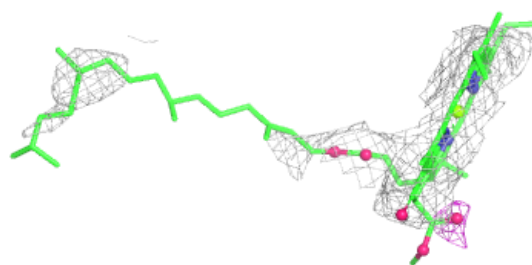


**Electron density around CLA C 1032:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

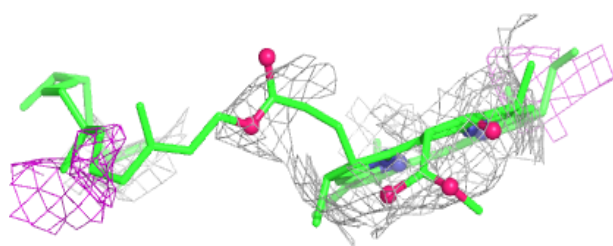
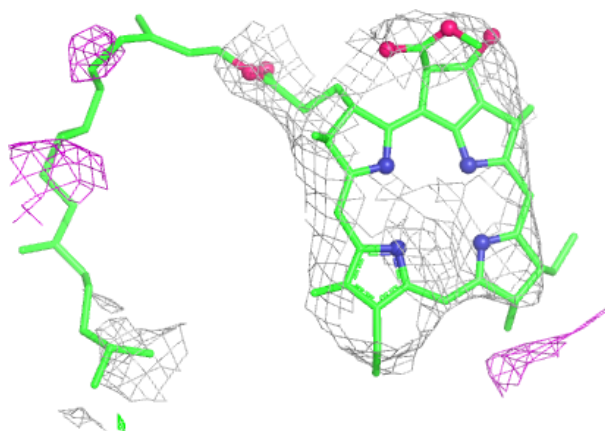
**Electron density around CLA b 6012:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

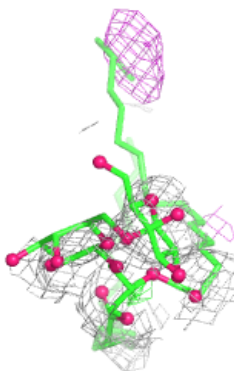
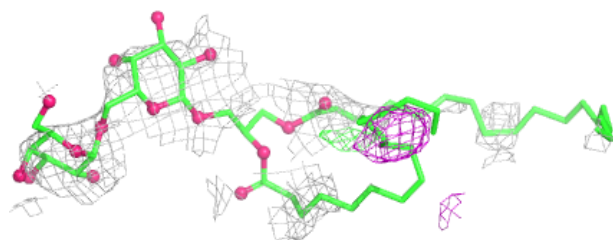
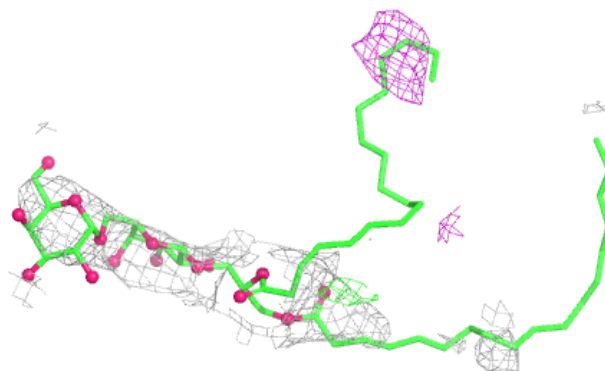


**Electron density around PHO a 6038:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

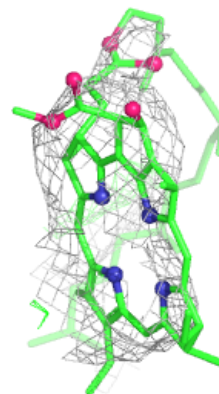
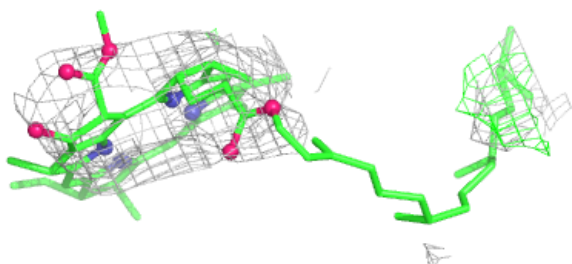
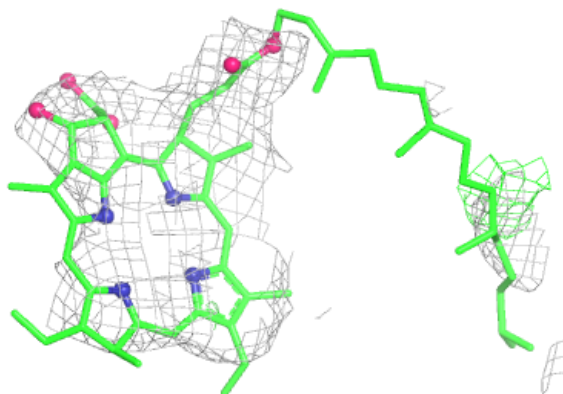
**Electron density around DGD b 6058:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

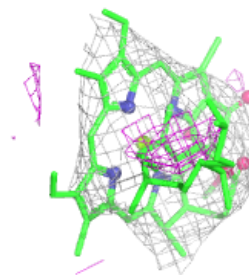
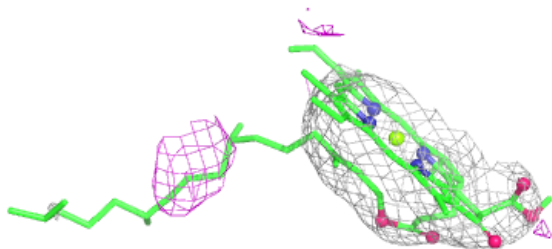
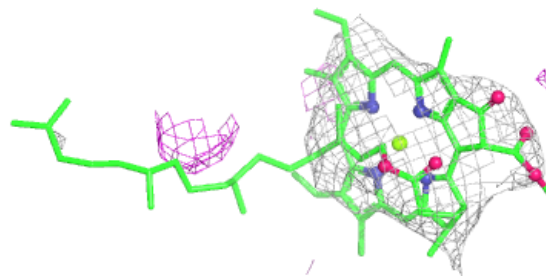


**Electron density around PHO d 6039:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

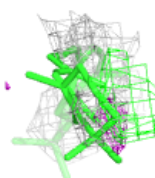
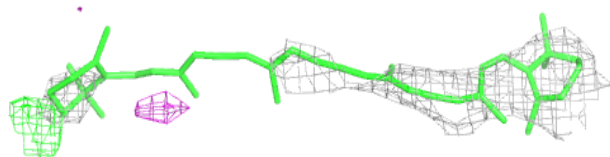
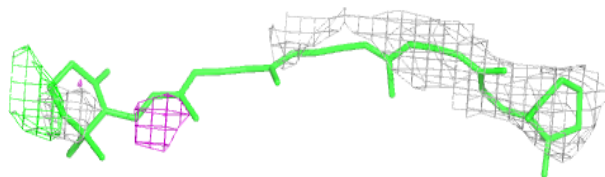
**Electron density around CLA C 1029:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

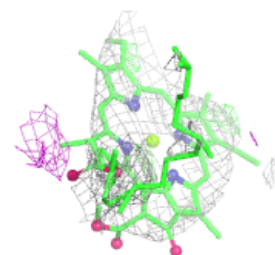
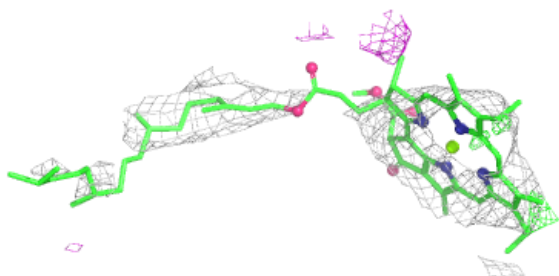
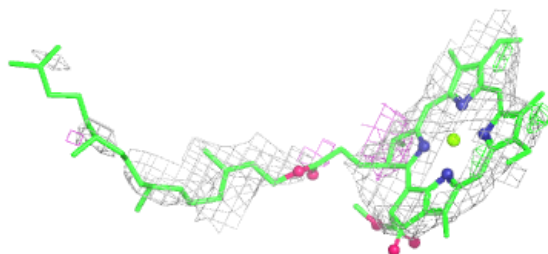


**Electron density around BCR C 1052:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

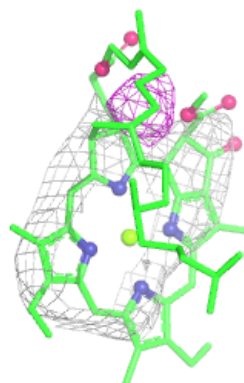
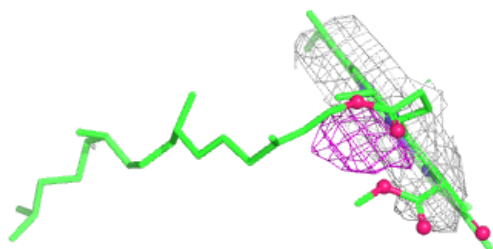
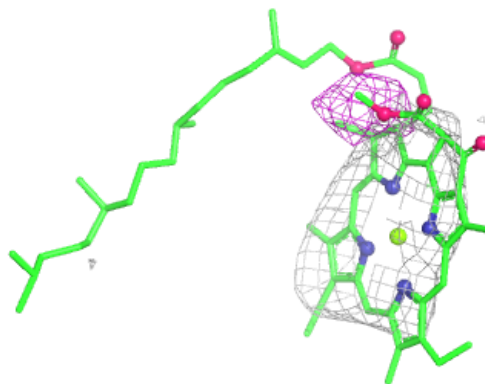
**Electron density around CLA a 6003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 6031:**

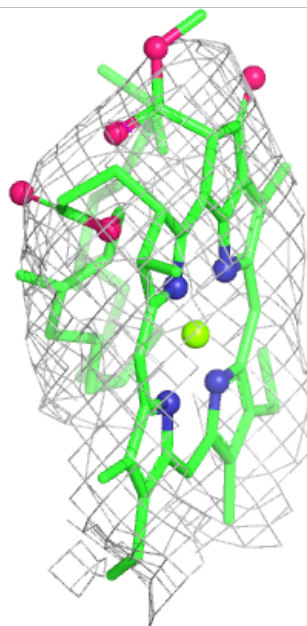
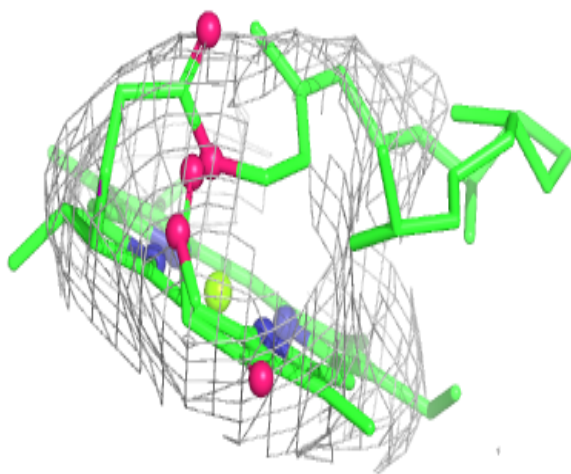
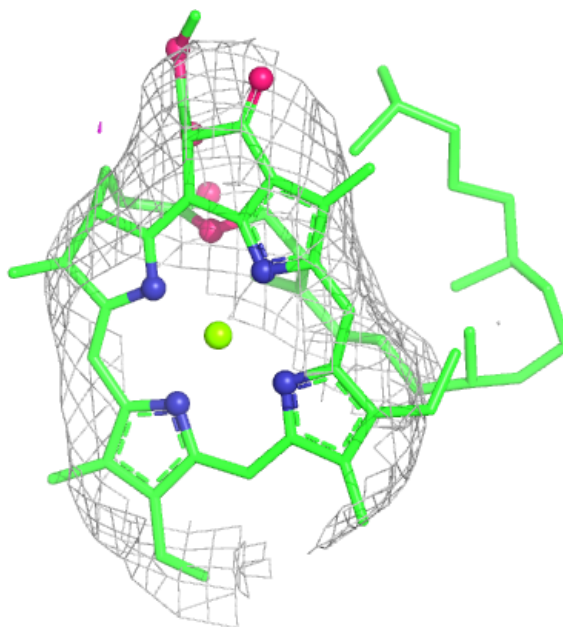
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





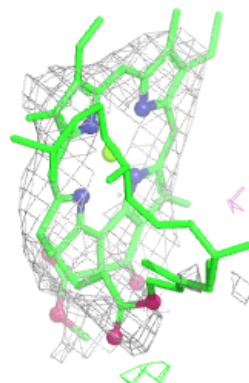
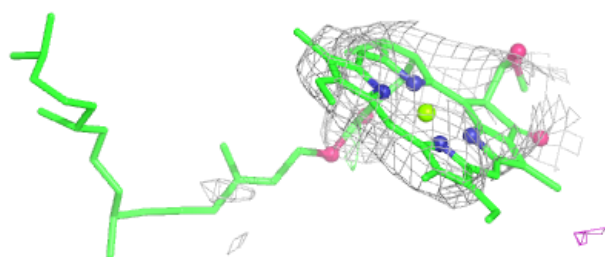
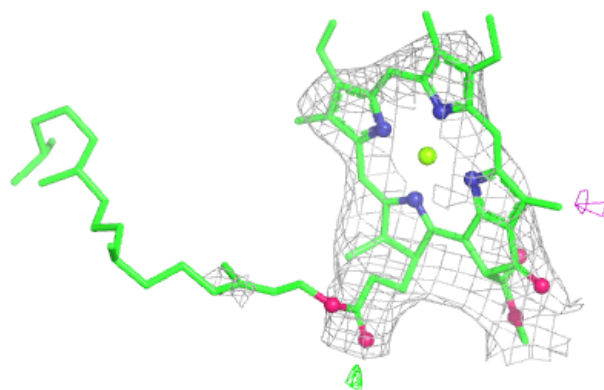
**Electron density around CLA b 6022:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

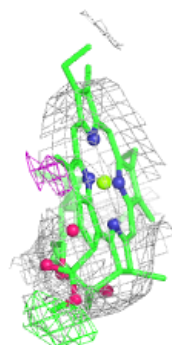
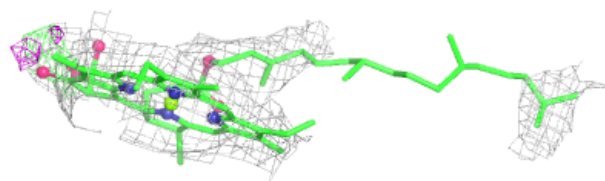
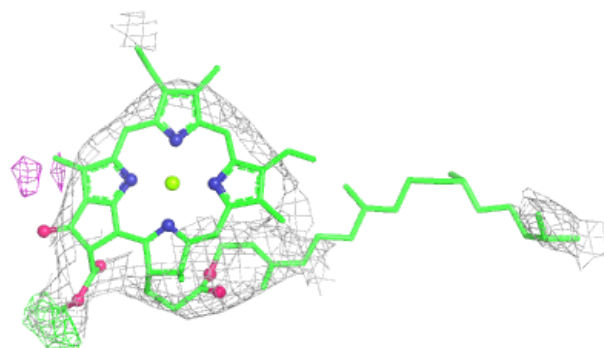


**Electron density around CLA D 1008:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

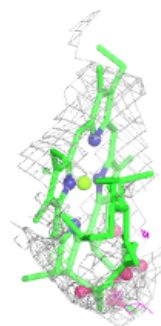
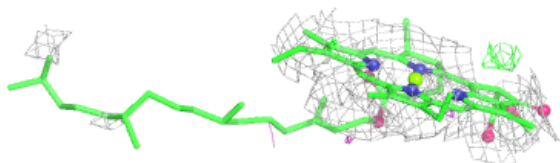
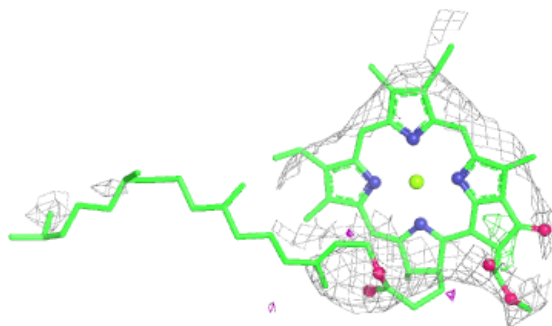
**Electron density around CLA B 1011:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



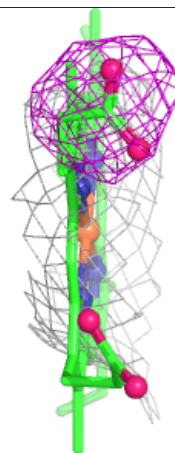
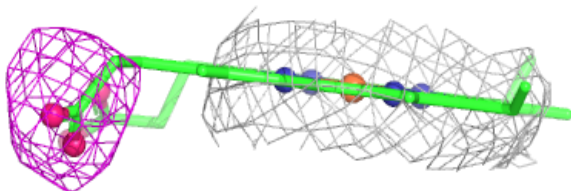
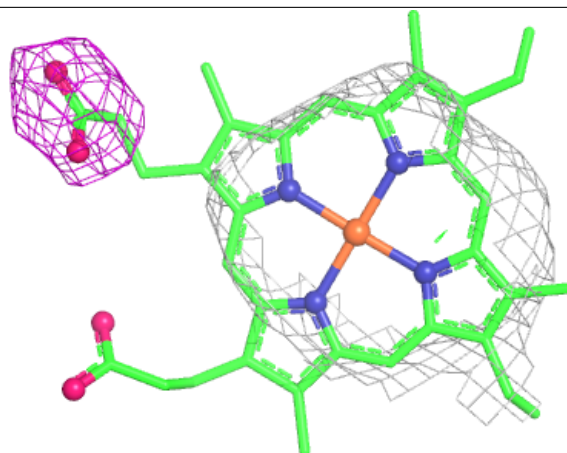
**Electron density around CLA b 6011:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

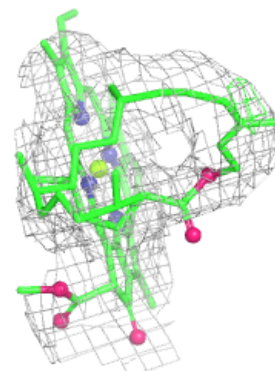
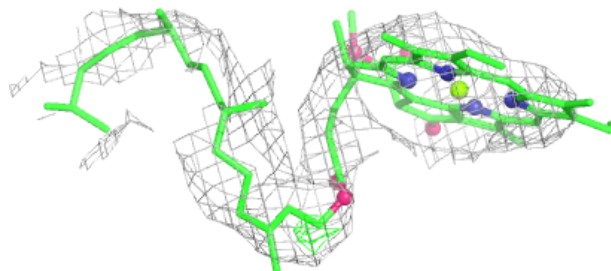
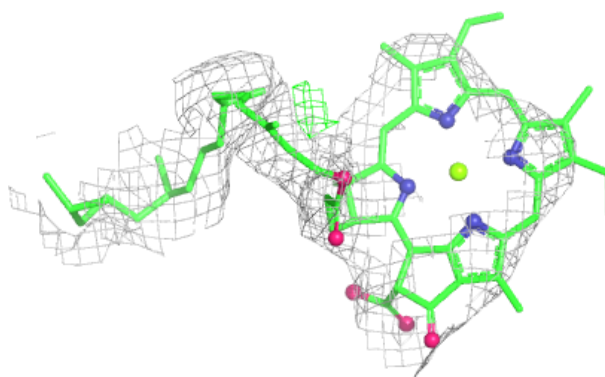


**Electron density around HEM f 6040:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

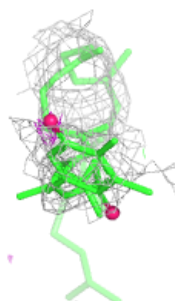
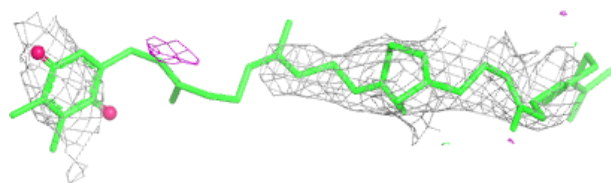
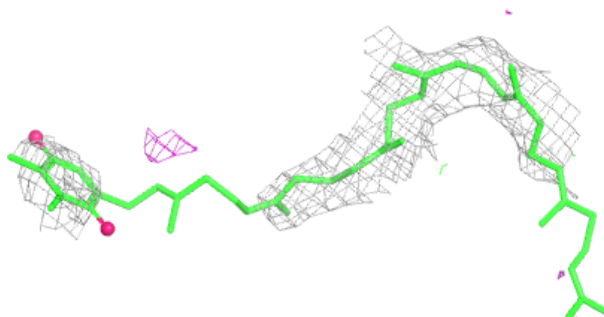
**Electron density around CLA a 6006:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

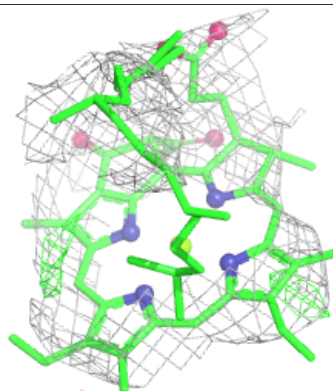
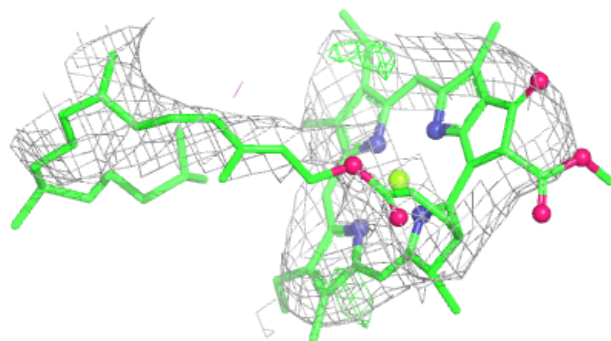
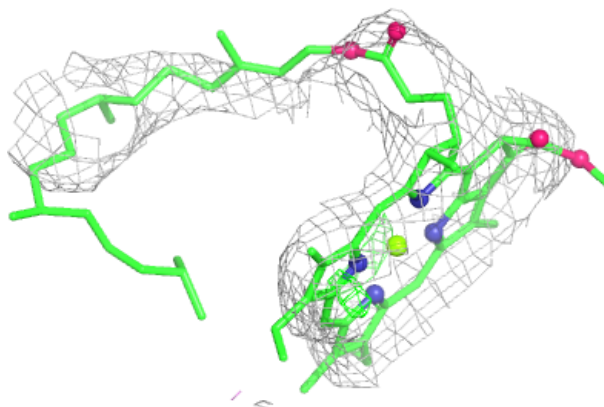


**Electron density around PQ9 D 1042:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

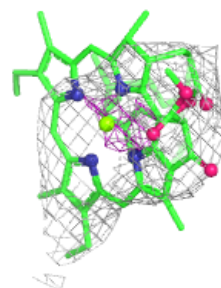
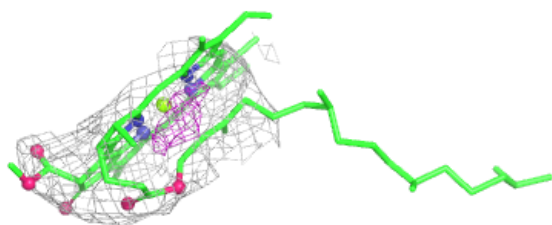
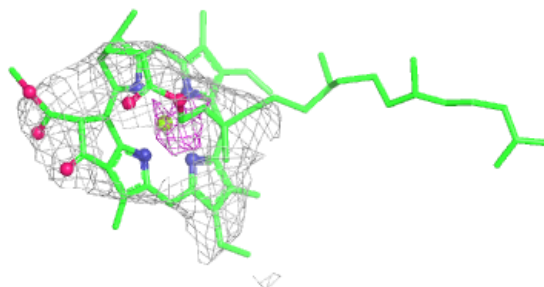
**Electron density around CLA c 6028:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

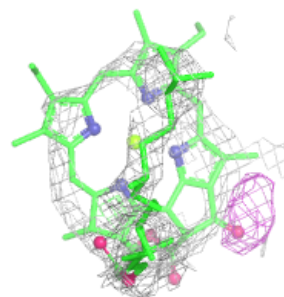
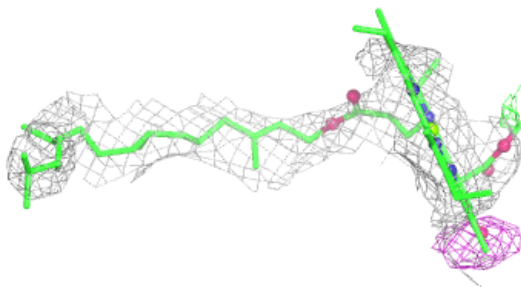
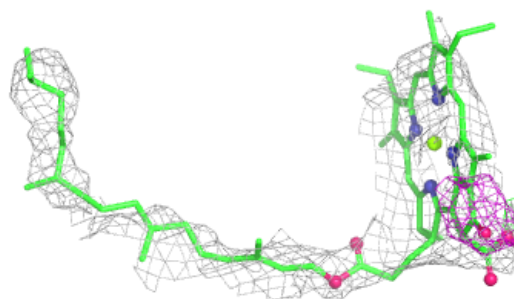


**Electron density around CLA c 6029:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA h 6017:**

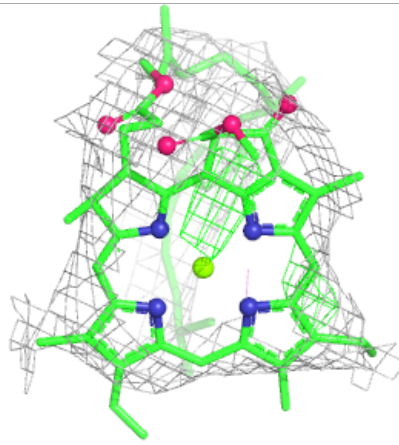
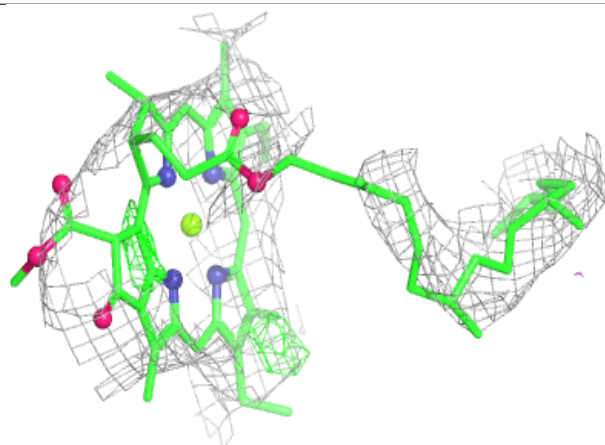
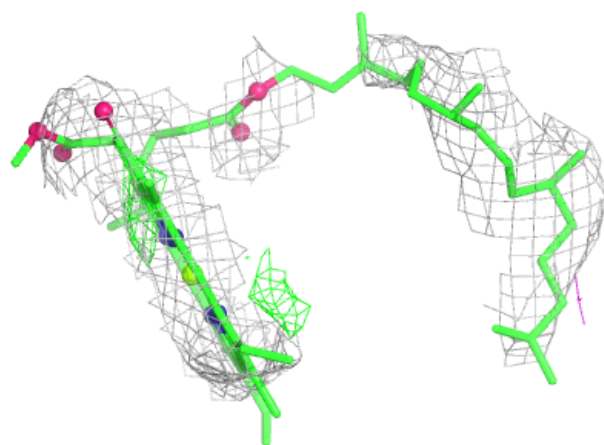
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 1019:**

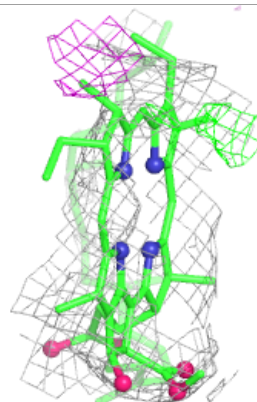
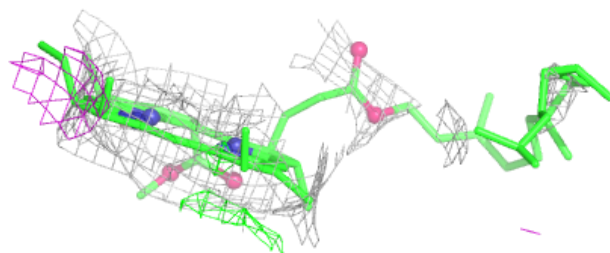
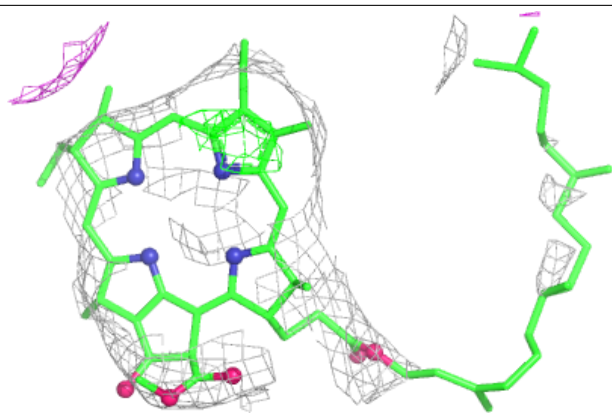
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



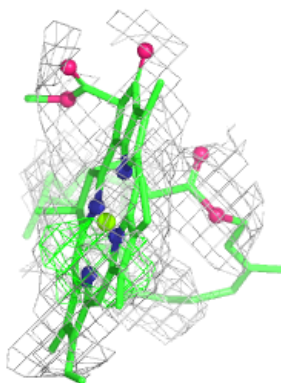
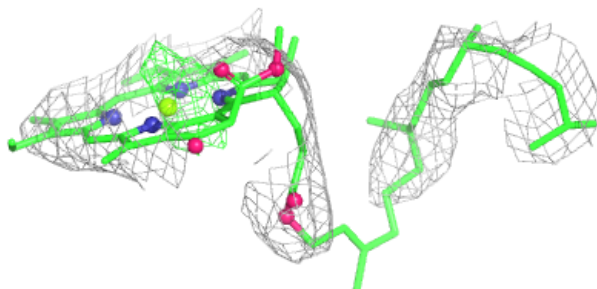
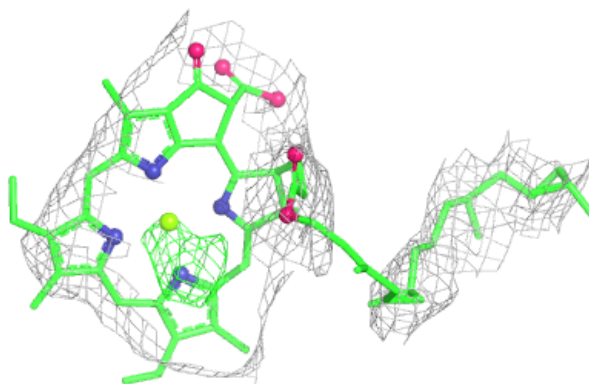


**Electron density around PHO A 1038:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

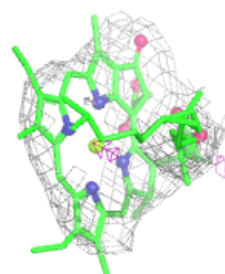
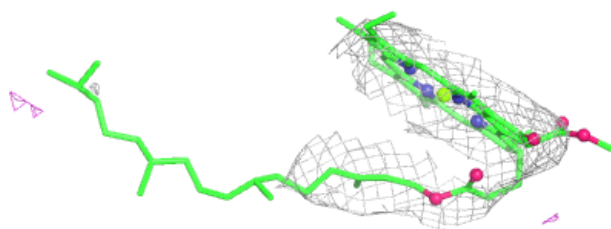
**Electron density around CLA A 1006:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

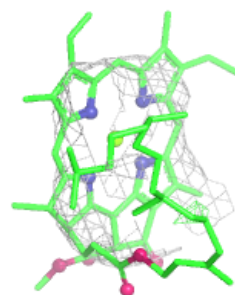
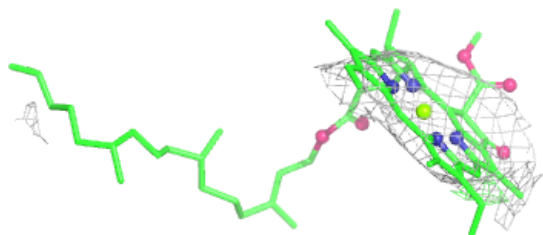


**Electron density around CLA b 6016:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

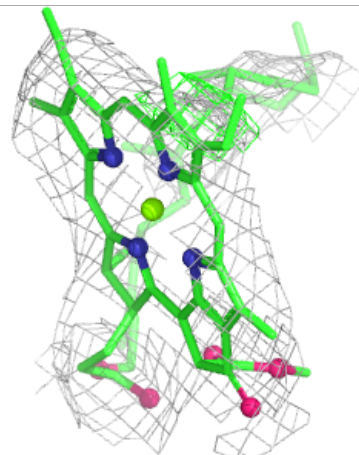
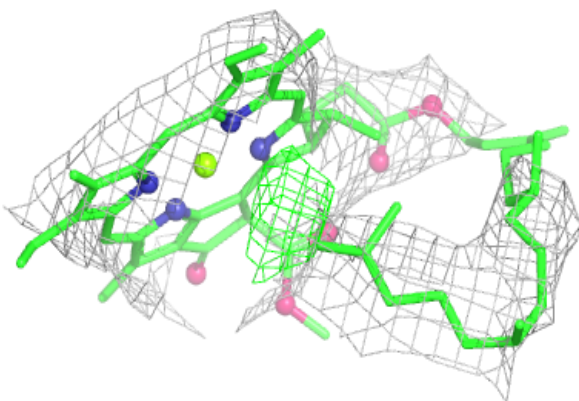
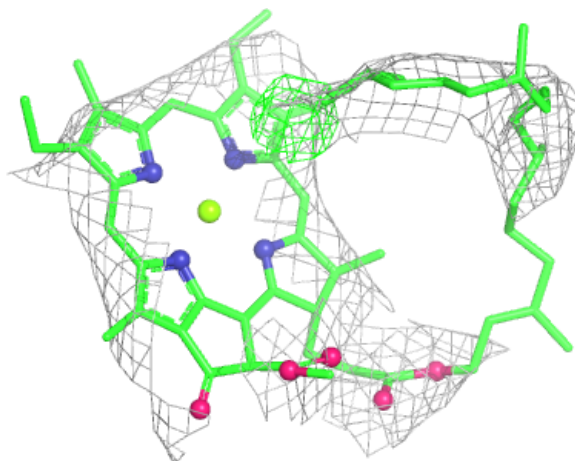
**Electron density around CLA C 1035:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



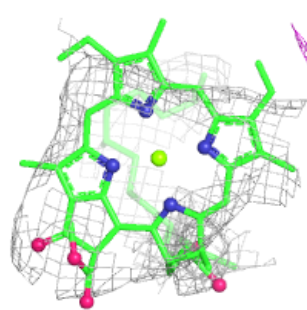
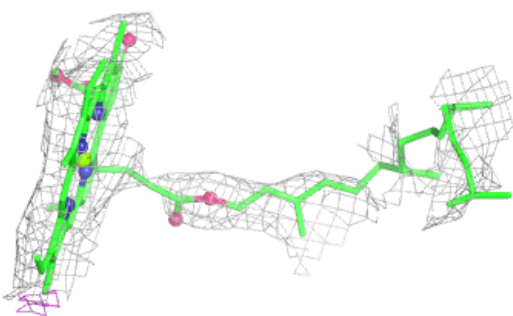
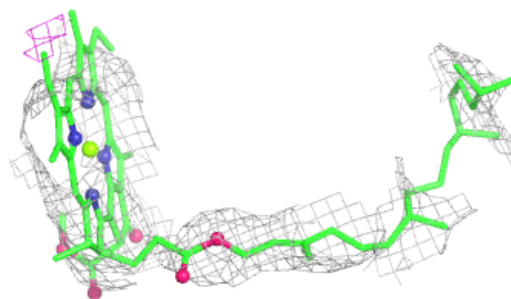
**Electron density around CLA B 1023:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

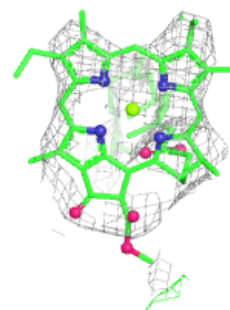
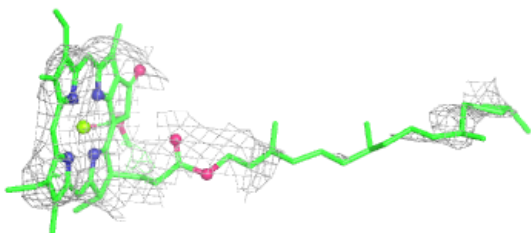
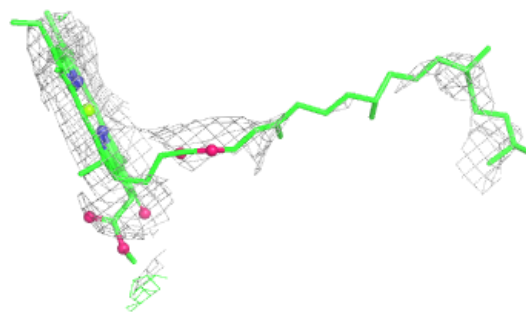


**Electron density around CLA c 6030:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

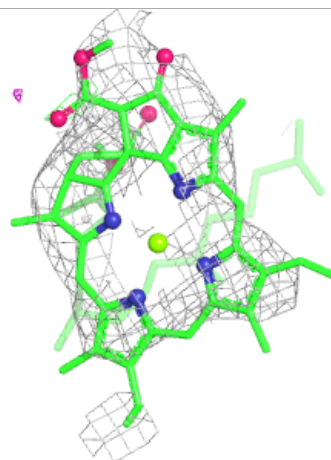
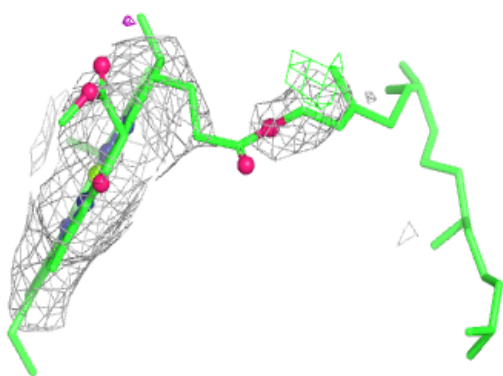
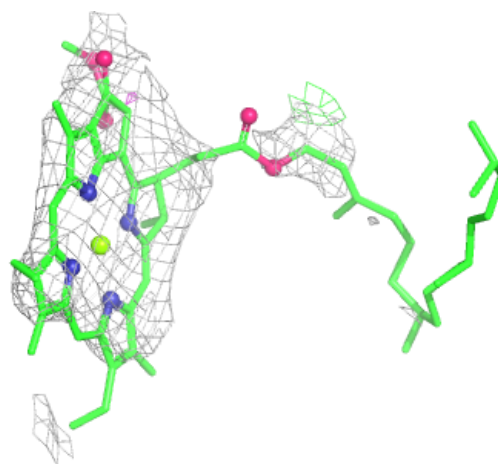
**Electron density around CLA B 1012:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



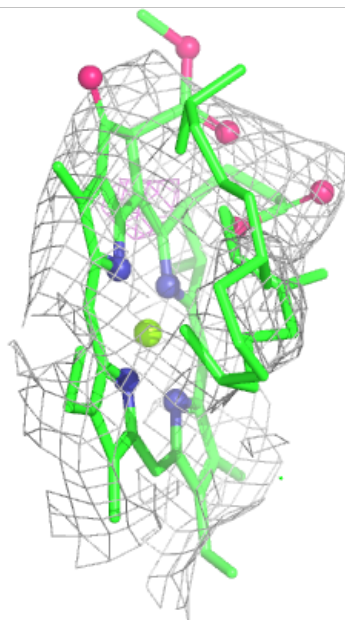
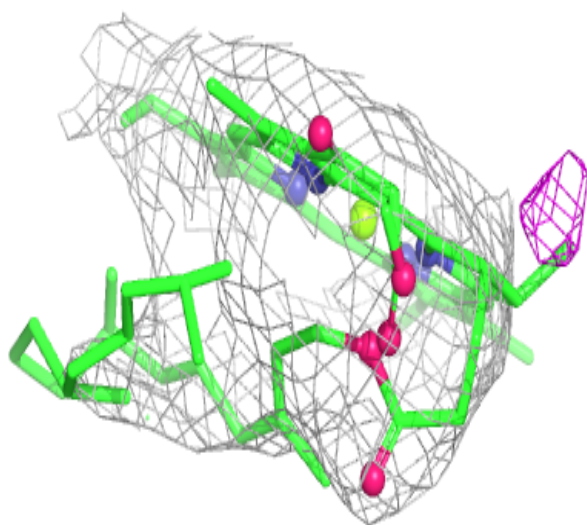
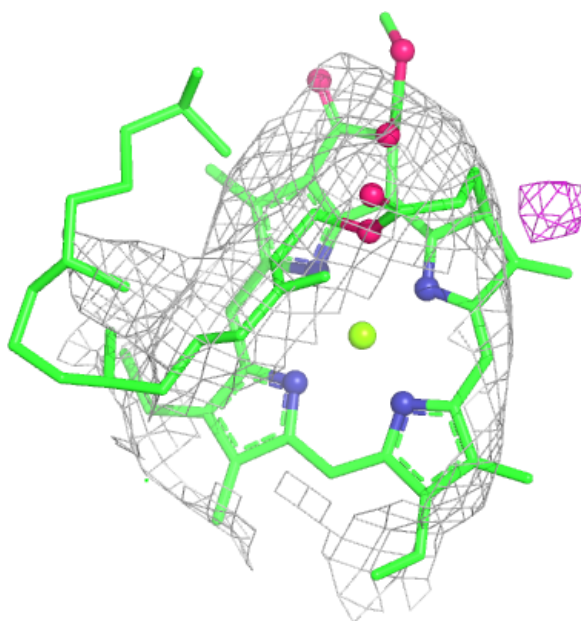
**Electron density around CLA A 1007:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1022:**

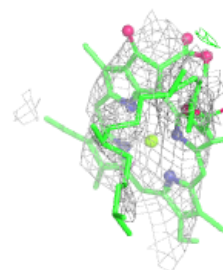
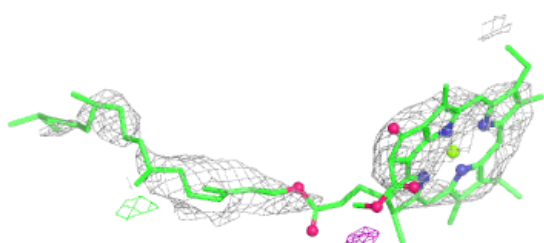
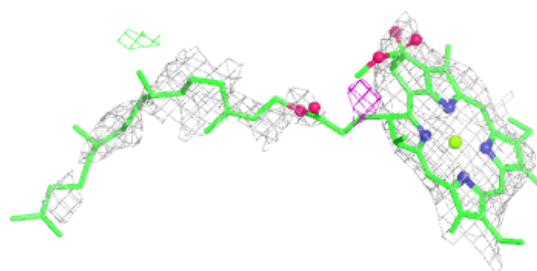
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



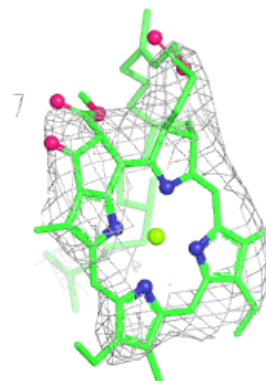
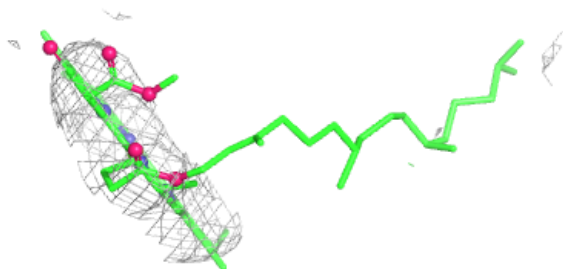
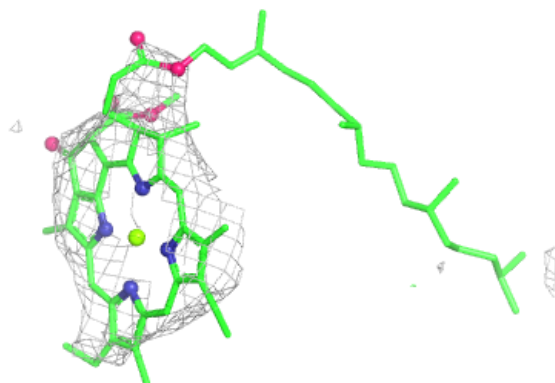


**Electron density around CLA A 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA C 1031:**

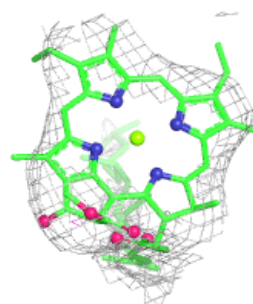
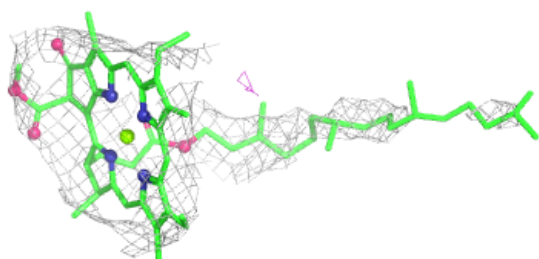
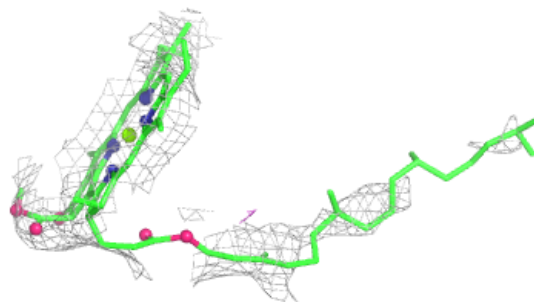
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



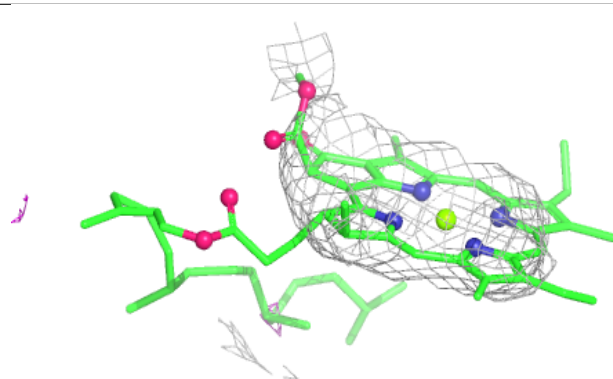
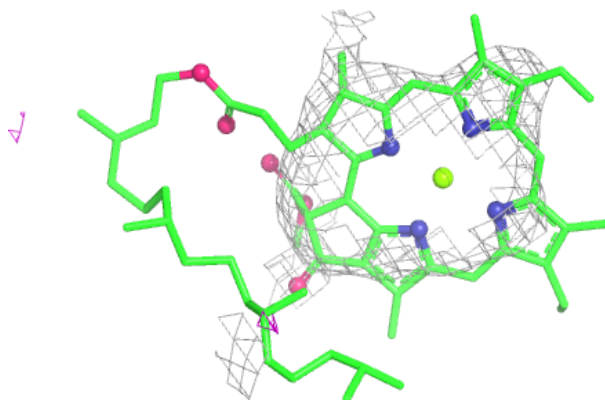


**Electron density around CLA B 1015:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

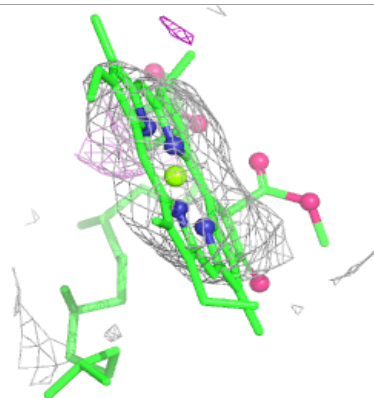
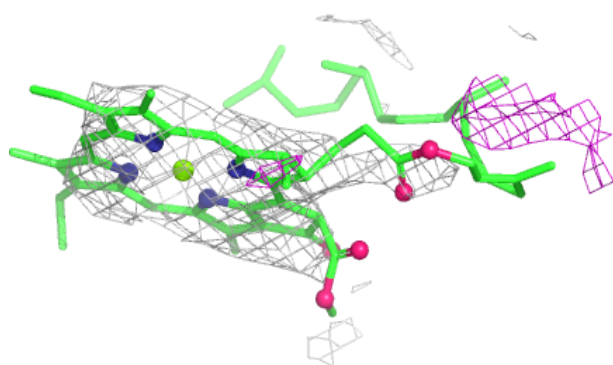
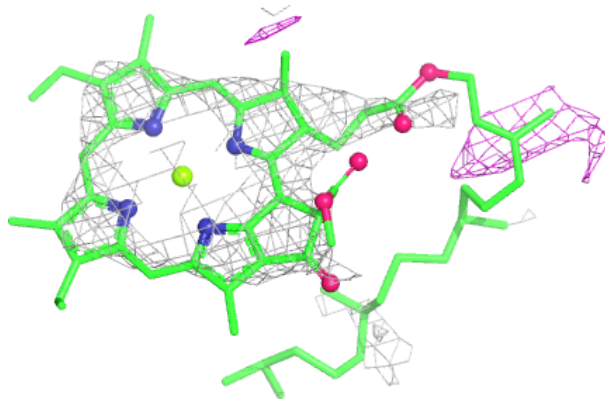
**Electron density around CLA c 6033:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

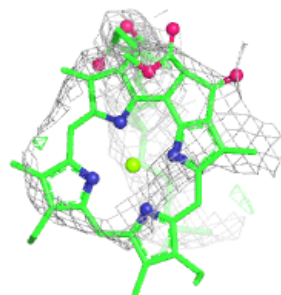
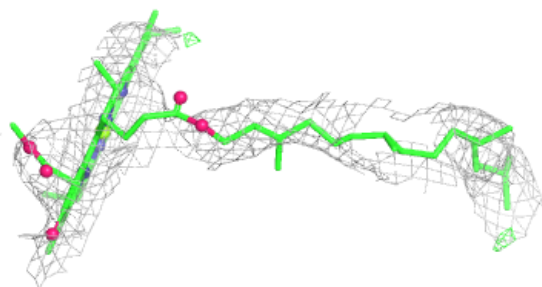
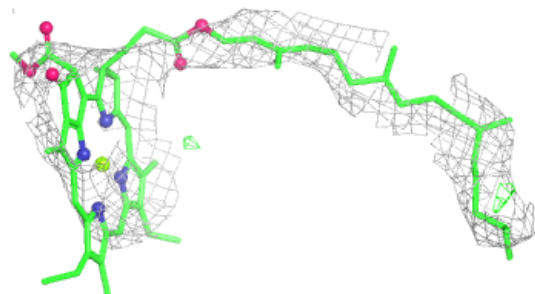


**Electron density around CLA C 1033:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

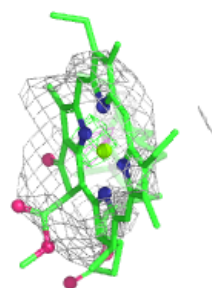
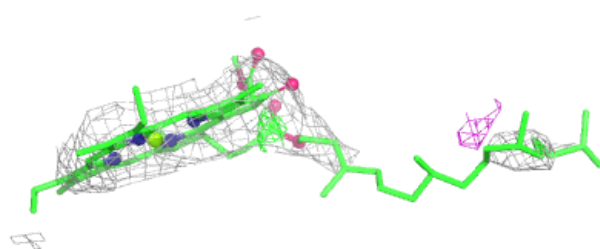
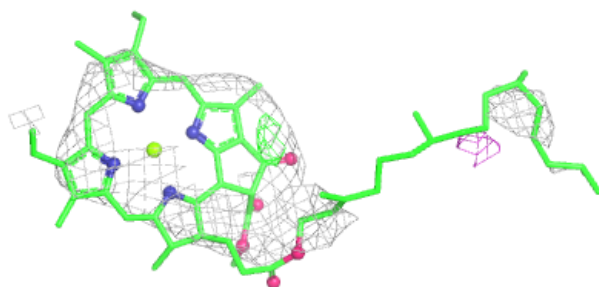
**Electron density around CLA H 1017:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



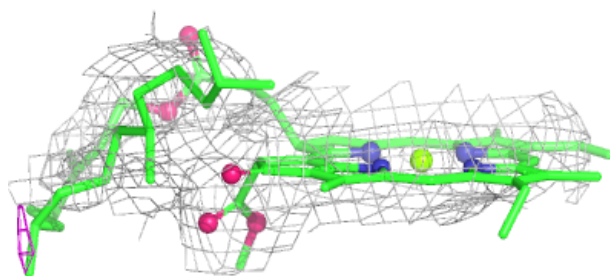
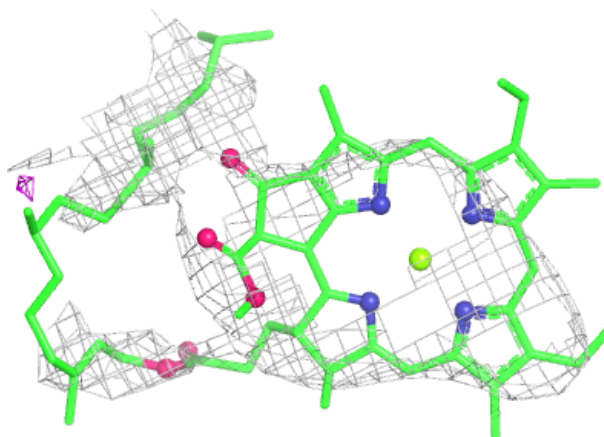
**Electron density around CLA B 1010:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



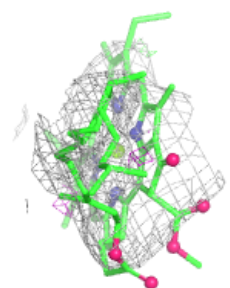
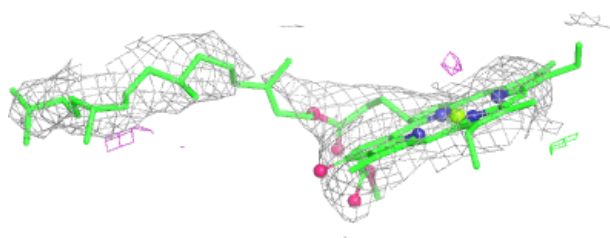
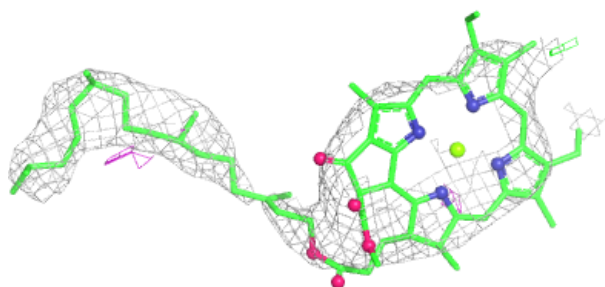
**Electron density around CLA b 6018:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

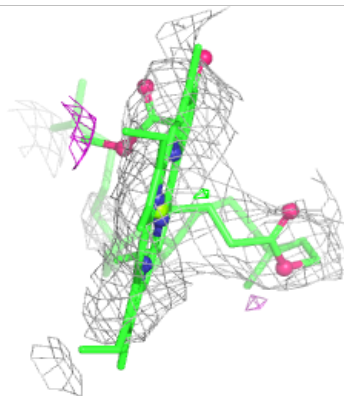
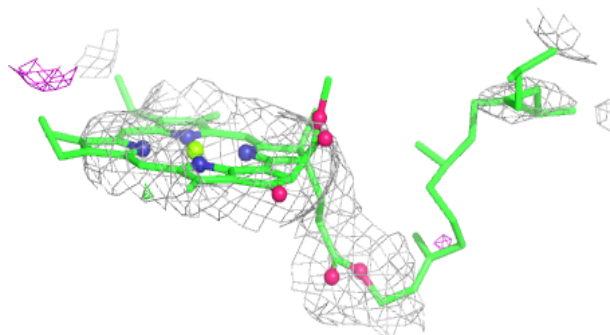
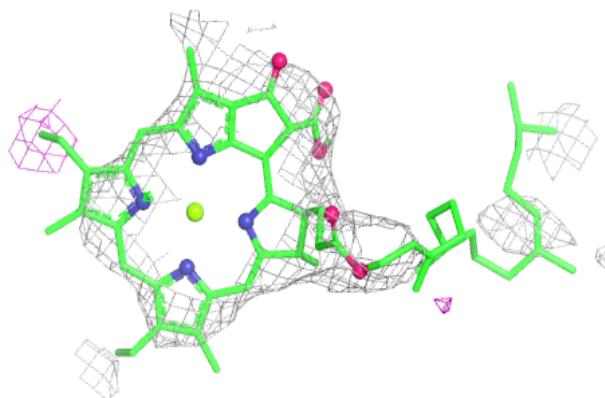


**Electron density around CLA b 6010:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

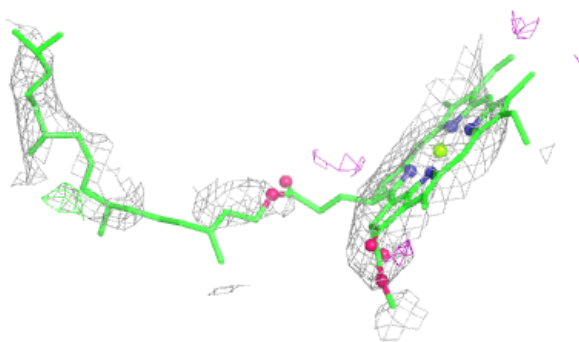
**Electron density around CLA b 6020:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

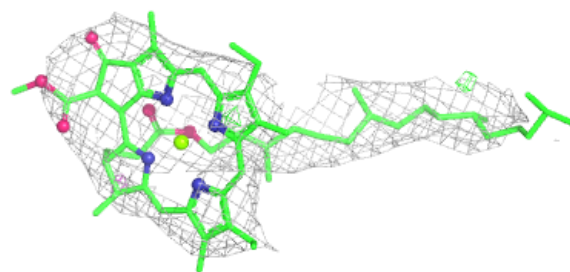


**Electron density around CLA D 1004:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

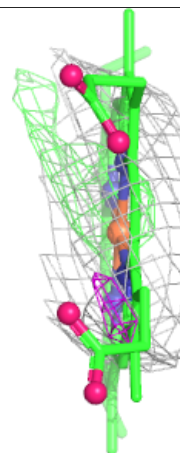
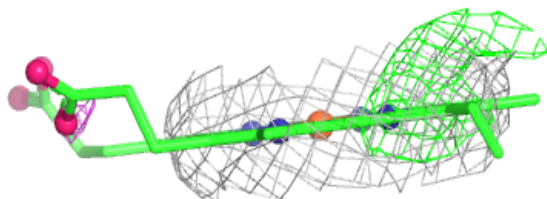
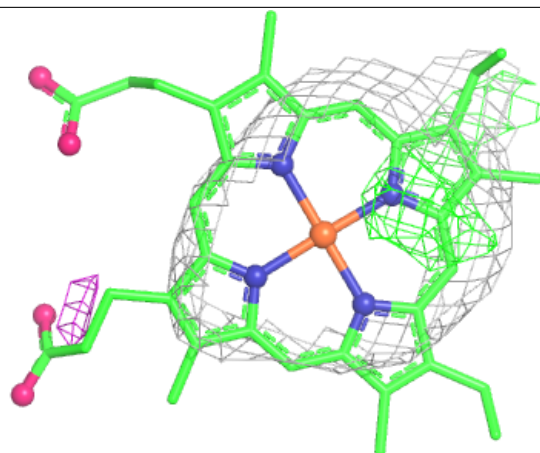
**Electron density around CLA B 1016:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM F 1040:**

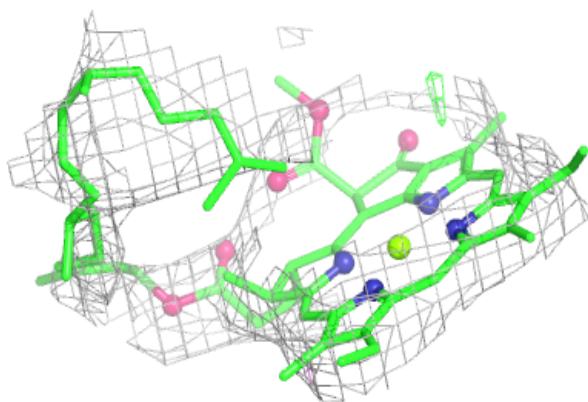
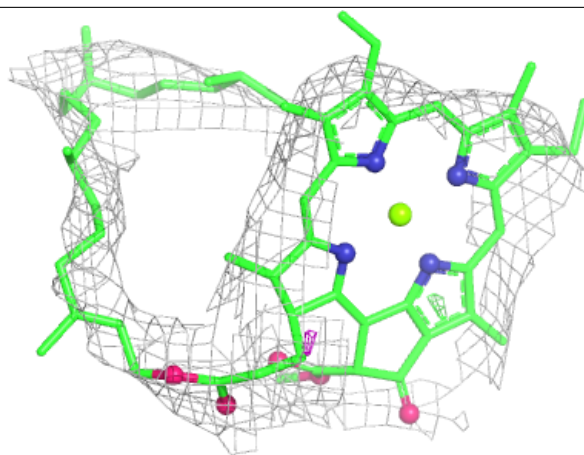
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





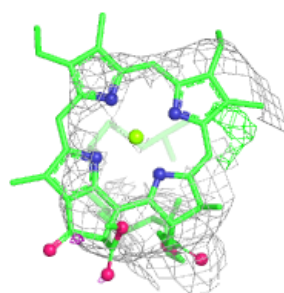
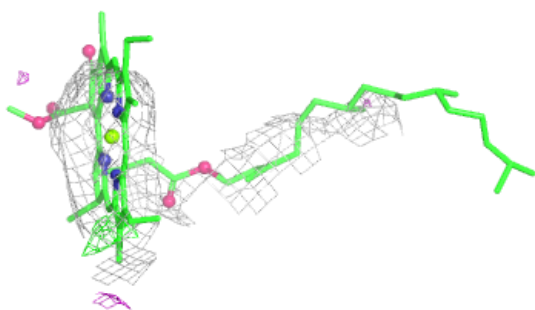
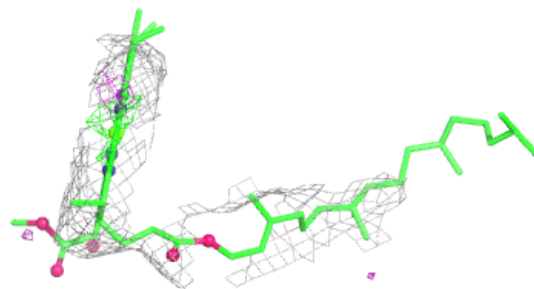
**Electron density around CLA b 6023:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

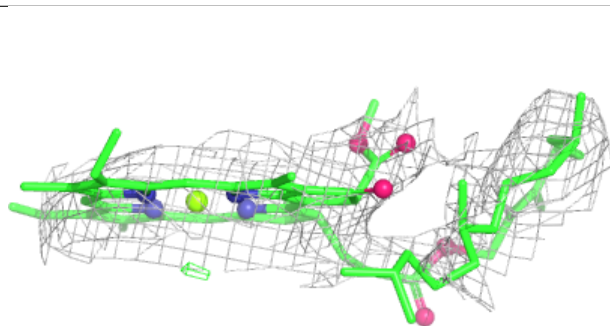
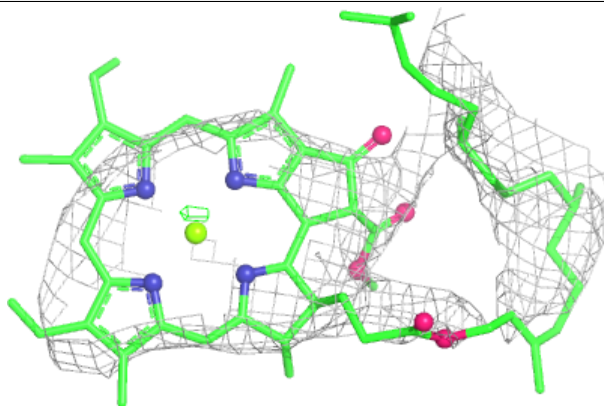


**Electron density around CLA b 6013:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

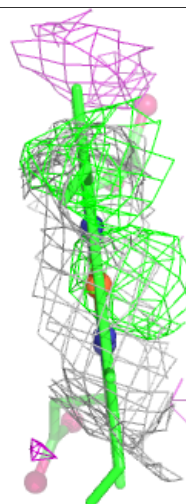
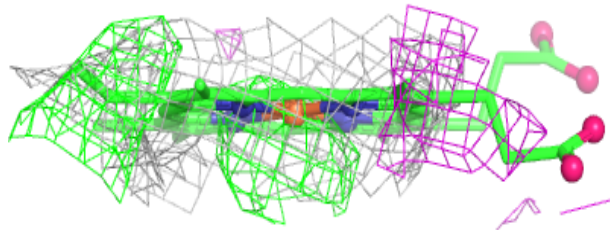
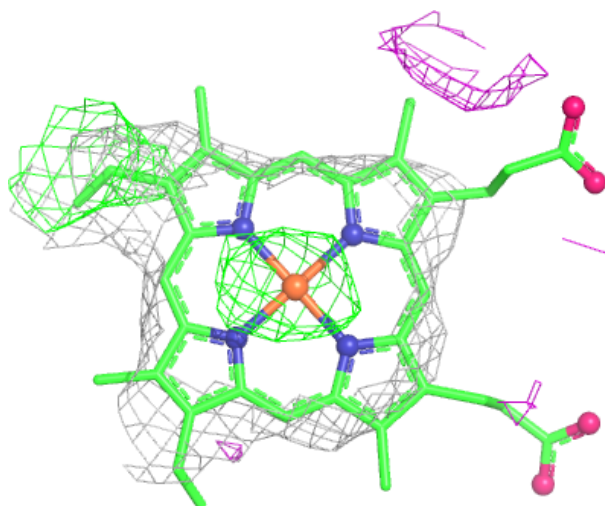
**Electron density around CLA B 1018:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



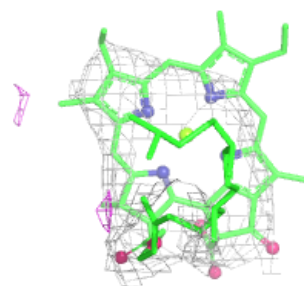
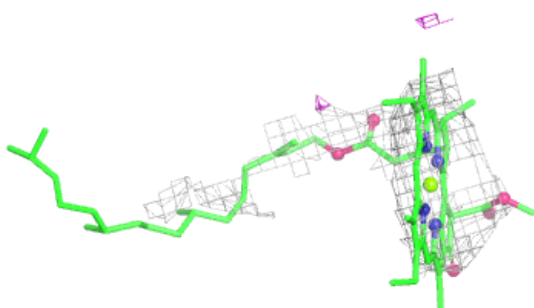
**Electron density around HEM V 1041:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



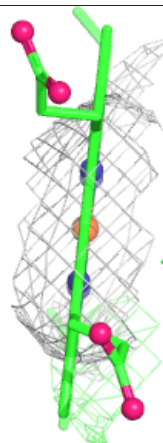
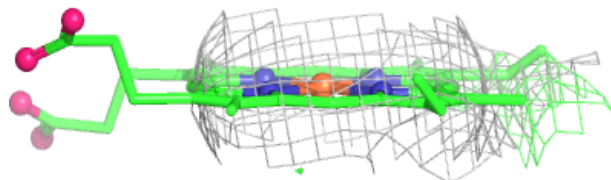
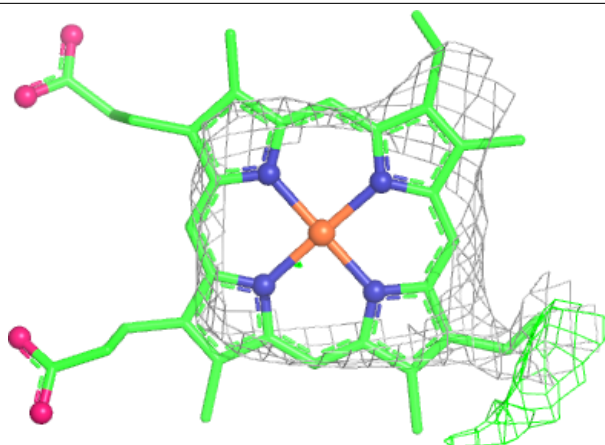
**Electron density around CLA B 1013:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



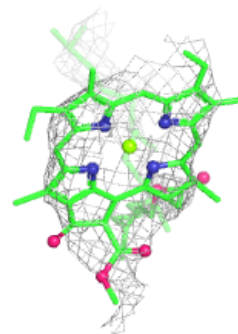
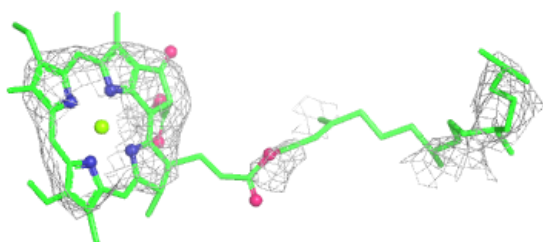
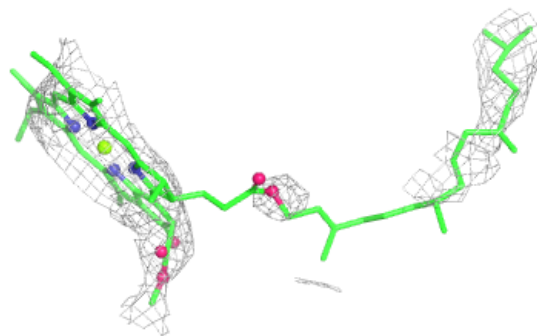
**Electron density around HEM v 6041:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

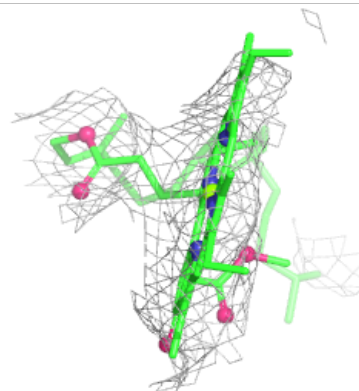
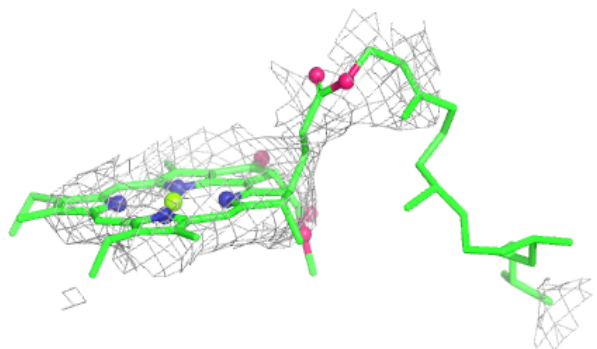
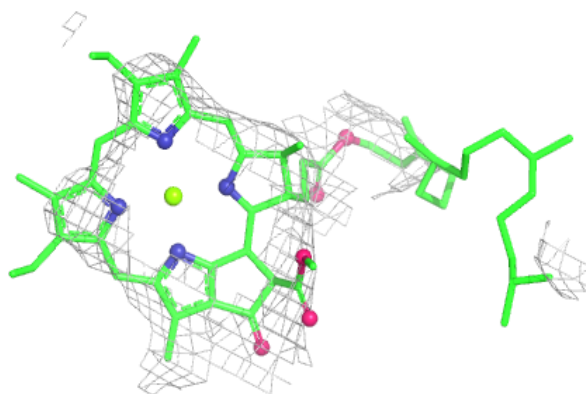


**Electron density around CLA d 6004:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 1020:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.