



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:42 AM GMT

PDB ID : 1KF6  
Title : E. coli Quinol-Fumarate Reductase with Bound Inhibitor HQNO  
Authors : Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.  
Deposited on : 2001-11-19  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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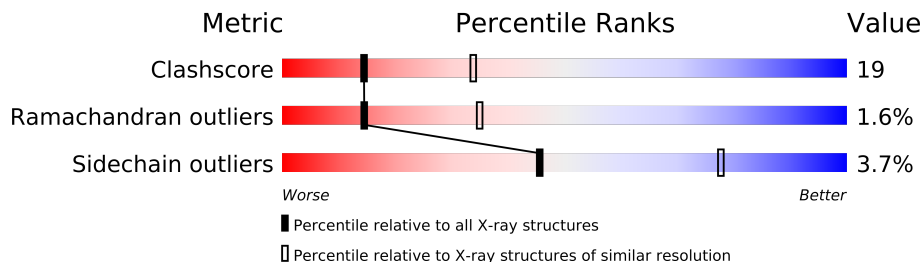
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 79885                       | 1939 (2.70-2.70)                                      |
| Ramachandran outliers | 78287                       | 1905 (2.70-2.70)                                      |
| Sidechain outliers    | 78261                       | 1905 (2.70-2.70)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 602    |                  |
| 1   | M     | 602    |                  |
| 2   | B     | 243    |                  |
| 2   | N     | 243    |                  |
| 3   | C     | 130    |                  |
| 3   | O     | 130    |                  |
| 4   | D     | 119    |                  |
| 4   | P     | 119    |                  |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 17071 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FUMARATE REDUCTASE FLAVOPROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4448  | 2775 | 802 | 840 | 31 |         |         |       |
| 1   | M     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4448  | 2775 | 802 | 840 | 31 |         |         |       |

- Molecule 2 is a protein called FUMARATE REDUCTASE IRON-SULFUR PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1888  | 1189 | 323 | 357 | 19 |         |         |       |
| 2   | N     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1888  | 1189 | 323 | 357 | 19 |         |         |       |

- Molecule 3 is a protein called FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1058  | 720 | 166 | 169 | 3 |         |         |       |
| 3   | O     | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1058  | 720 | 166 | 169 | 3 |         |         |       |

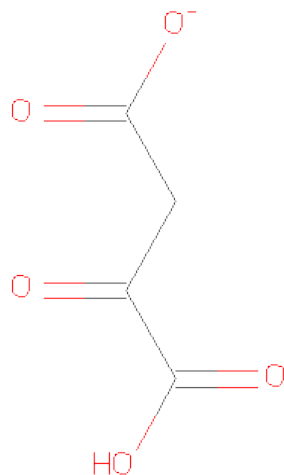
- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 626 | 151 | 142 | 7 |         |         |       |
| 4   | P     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 626 | 151 | 142 | 7 |         |         |       |

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 5   | A     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 5   | M     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula:  $C_4H_3O_5$ ).



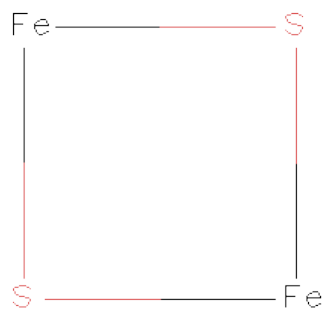
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 9     | 4 | 5 |         |         |
| 6   | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 9     | 4 | 5 |         |         |

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 7   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 7   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



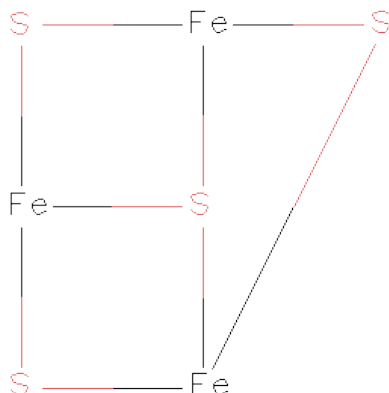
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

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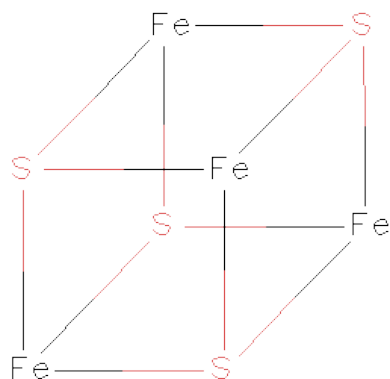
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8   | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



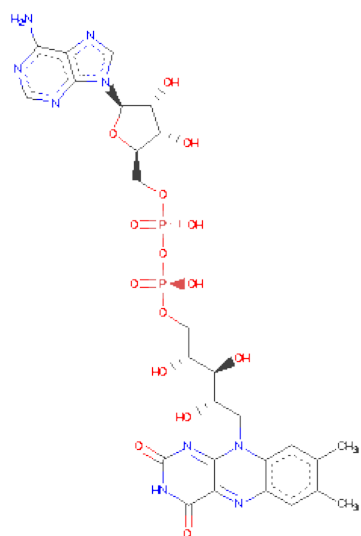
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |
| 9   | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 10  | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 10  | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 11 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



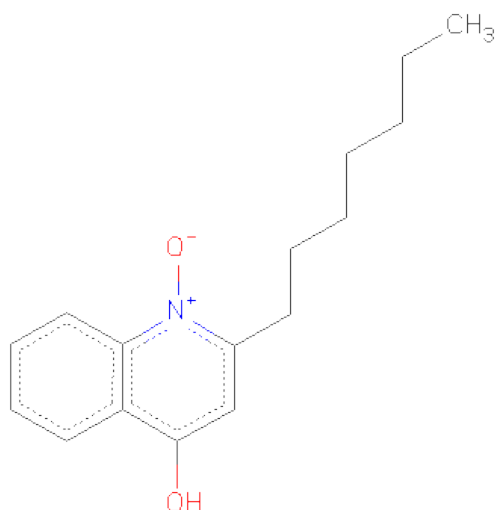
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 11  | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 11  | M     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

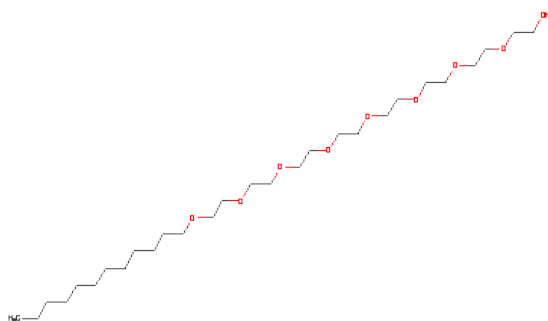
- Molecule 12 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula:  $C_{16}H_{21}NO_2$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 12  | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 16 | 1 | 2 |         |         |
| 12  | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 16 | 1 | 2 |         |         |

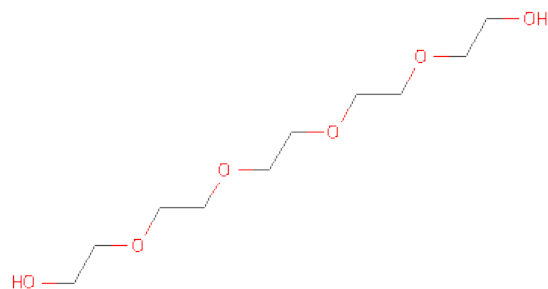
- Molecule 13 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula:  $C_{28}H_{58}O_9$ ).





| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 13  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |
| 13  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |
| 13  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |
| 13  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |
| 13  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |

- Molecule 14 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 14  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |

- Molecule 15 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | A     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 15  | B     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | M     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 15  | N     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

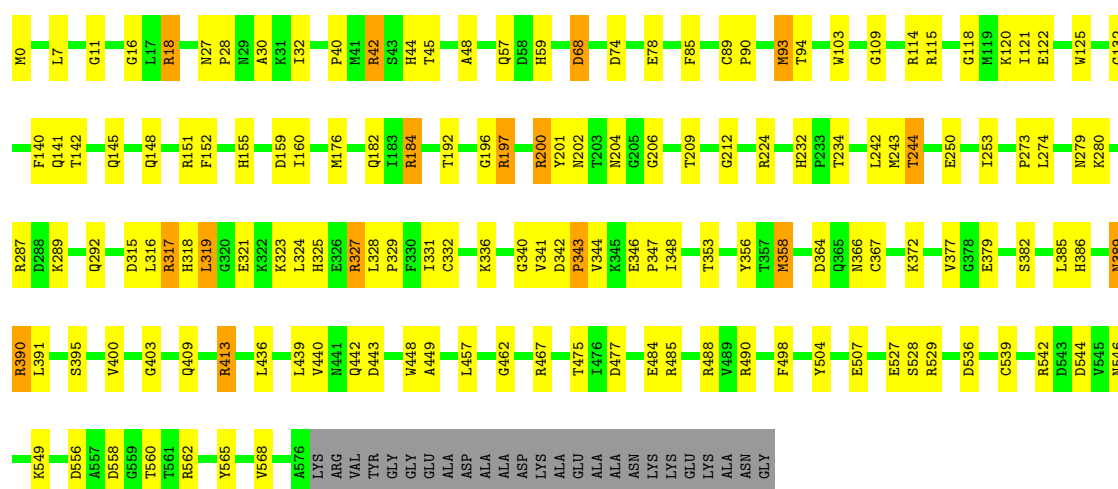
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

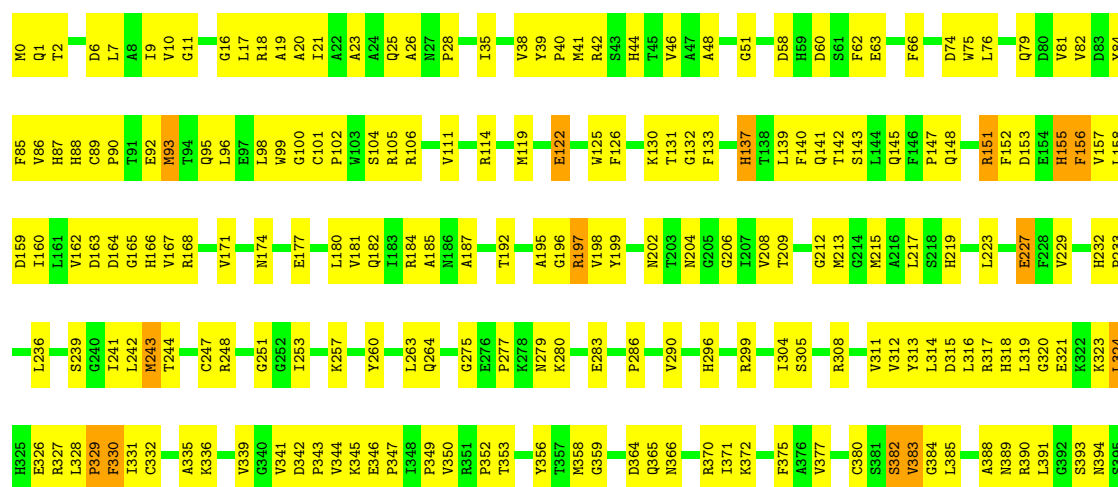
#### • Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN

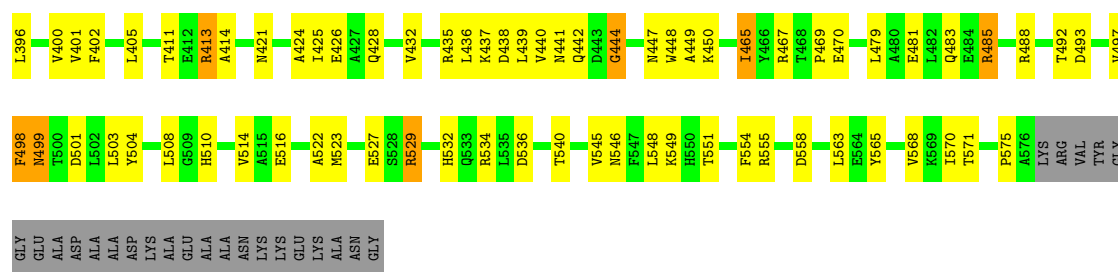
Chain A:



#### • Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN

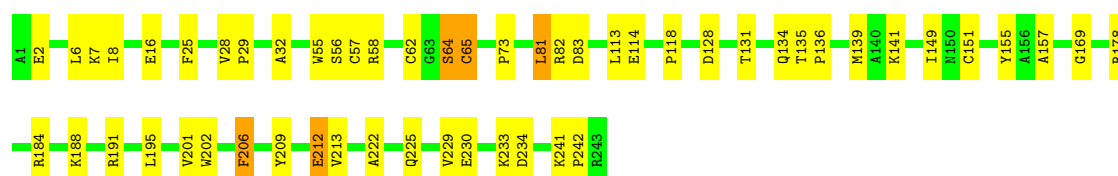
Chain M:





• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain B:



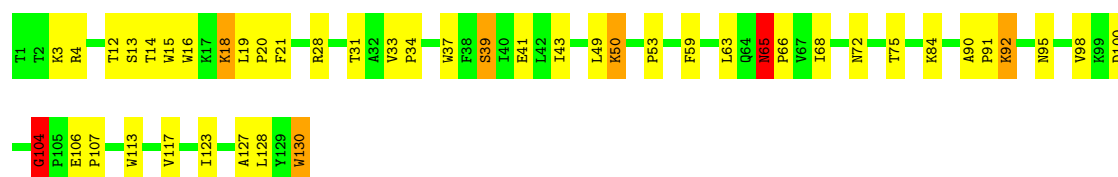
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain N:



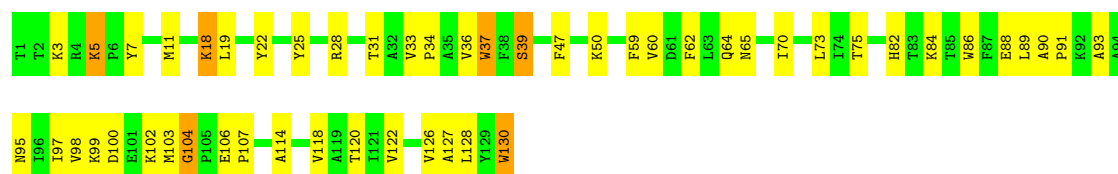
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain C:



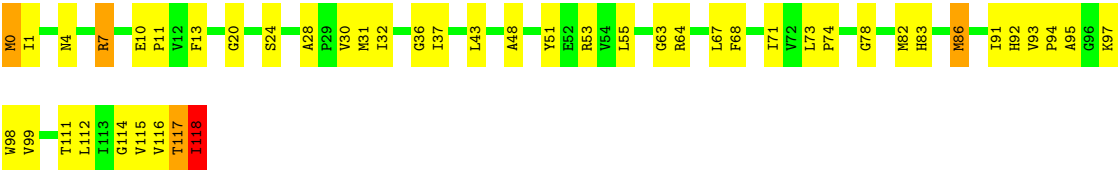
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain O:



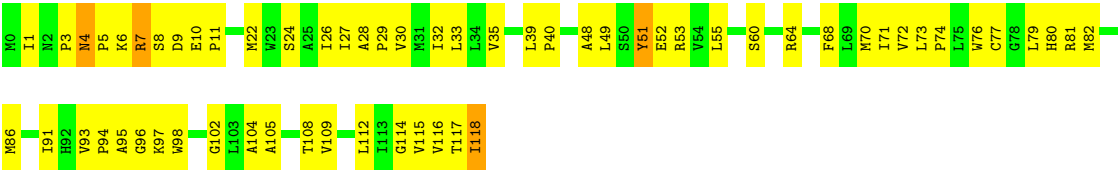
• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain D:



● Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain P:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | P 21 21 21                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 96.50Å 137.84Å 273.45Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 20.00 – 2.70                                   | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (20.00-2.70)                   | Depositor |
| $R_{merge}$  | (Not available)                                | Depositor |
| $R_{sym}$  | (Not available)                                | Depositor |
| Refinement program                                       | CNS, REFMAC                                    | Depositor |
| R, $R_{free}$  | 0.231 , 0.280                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 17071  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 55.0   | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, SF4, ACT, 1PE, F3S, FES, CE1, HQO, K, FAD

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     | 0.81         | 0/4540          | 0.98        | 10/6139 (0.2%)  |
| 1   | M     | 0.53         | 1/4540 (0.0%)   | 0.81        | 2/6139 (0.0%)   |
| 2   | B     | 0.78         | 1/1931 (0.1%)   | 0.92        | 7/2617 (0.3%)   |
| 2   | N     | 0.59         | 0/1931          | 0.81        | 1/2617 (0.0%)   |
| 3   | C     | 0.77         | 3/1094 (0.3%)   | 0.87        | 2/1496 (0.1%)   |
| 3   | O     | 0.68         | 3/1094 (0.3%)   | 0.79        | 1/1496 (0.1%)   |
| 4   | D     | 0.78         | 1/956 (0.1%)    | 0.89        | 1/1303 (0.1%)   |
| 4   | P     | 0.70         | 2/956 (0.2%)    | 0.82        | 0/1303          |
| All | All   | 0.70         | 11/17042 (0.1%) | 0.88        | 24/23110 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | C     | 0                   | 2                   |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | D     | 118 | ILE  | C-OXT | 11.65 | 1.45        | 1.23     |
| 4   | P     | 118 | ILE  | C-OXT | 8.01  | 1.38        | 1.23     |
| 2   | B     | 65  | CYS  | CB-SG | -7.99 | 1.68        | 1.82     |
| 3   | C     | 65  | ASN  | C-O   | -7.42 | 1.09        | 1.23     |
| 3   | O     | 104 | GLY  | C-O   | -6.55 | 1.13        | 1.23     |
| 4   | P     | 118 | ILE  | CA-CB | 6.31  | 1.69        | 1.54     |
| 3   | C     | 130 | TRP  | C-OXT | 6.25  | 1.35        | 1.23     |
| 3   | O     | 130 | TRP  | CA-CB | 6.17  | 1.67        | 1.53     |
| 3   | O     | 65  | ASN  | C-O   | -5.51 | 1.12        | 1.23     |
| 1   | M     | 359 | GLY  | C-O   | 5.23  | 1.32        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | C     | 104 | GLY  | CA-C  | -5.09 | 1.43        | 1.51     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 485 | ARG  | NE-CZ-NH2 | -7.24 | 116.68      | 120.30   |
| 4   | D     | 7   | ARG  | NE-CZ-NH2 | -7.24 | 116.68      | 120.30   |
| 2   | B     | 191 | ARG  | NE-CZ-NH1 | -6.88 | 116.86      | 120.30   |
| 3   | C     | 28  | ARG  | NE-CZ-NH2 | -6.71 | 116.95      | 120.30   |
| 2   | B     | 65  | CYS  | N-CA-CB   | -6.56 | 98.79       | 110.60   |
| 1   | M     | 151 | ARG  | NE-CZ-NH2 | -6.52 | 117.04      | 120.30   |
| 1   | A     | 477 | ASP  | CB-CG-OD1 | 6.42  | 124.08      | 118.30   |
| 1   | A     | 18  | ARG  | NE-CZ-NH1 | 6.12  | 123.36      | 120.30   |
| 1   | A     | 114 | ARG  | NE-CZ-NH2 | -5.93 | 117.33      | 120.30   |
| 1   | A     | 18  | ARG  | NE-CZ-NH2 | -5.88 | 117.36      | 120.30   |
| 2   | B     | 184 | ARG  | NE-CZ-NH2 | -5.86 | 117.37      | 120.30   |
| 1   | A     | 467 | ARG  | NE-CZ-NH2 | -5.83 | 117.39      | 120.30   |
| 2   | B     | 64  | SER  | C-N-CA    | 5.76  | 136.09      | 121.70   |
| 1   | M     | 529 | ARG  | NE-CZ-NH2 | -5.58 | 117.51      | 120.30   |
| 2   | B     | 65  | CYS  | N-CA-C    | 5.56  | 126.00      | 111.00   |
| 2   | B     | 65  | CYS  | CB-CA-C   | -5.54 | 99.32       | 110.40   |
| 3   | C     | 28  | ARG  | NE-CZ-NH1 | 5.51  | 123.05      | 120.30   |
| 1   | A     | 364 | ASP  | CB-CG-OD1 | 5.47  | 123.22      | 118.30   |
| 2   | B     | 83  | ASP  | CB-CG-OD2 | 5.25  | 123.02      | 118.30   |
| 1   | A     | 317 | ARG  | NE-CZ-NH1 | 5.23  | 122.91      | 120.30   |
| 1   | A     | 390 | ARG  | NE-CZ-NH2 | 5.18  | 122.89      | 120.30   |
| 2   | N     | 191 | ARG  | NE-CZ-NH2 | -5.08 | 117.76      | 120.30   |
| 3   | O     | 104 | GLY  | CA-C-O    | -5.06 | 111.49      | 120.60   |
| 1   | A     | 68  | ASP  | CB-CG-OD2 | -5.00 | 113.80      | 118.30   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 3   | C     | 65  | ASN  | Mainchain,Peptide |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,



and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4448  | 0        | 4335     | 119     | 0            |
| 1   | M     | 4448  | 0        | 4335     | 253     | 0            |
| 2   | B     | 1888  | 0        | 1837     | 44      | 0            |
| 2   | N     | 1888  | 0        | 1837     | 108     | 0            |
| 3   | C     | 1058  | 0        | 1108     | 47      | 0            |
| 3   | O     | 1058  | 0        | 1108     | 48      | 0            |
| 4   | D     | 926   | 0        | 971      | 47      | 0            |
| 4   | P     | 926   | 0        | 971      | 65      | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | M     | 1     | 0        | 0        | 0       | 0            |
| 6   | A     | 9     | 0        | 2        | 2       | 0            |
| 6   | M     | 9     | 0        | 2        | 0       | 0            |
| 7   | A     | 4     | 0        | 3        | 0       | 0            |
| 7   | B     | 4     | 0        | 3        | 0       | 0            |
| 7   | N     | 4     | 0        | 3        | 2       | 0            |
| 8   | B     | 4     | 0        | 0        | 0       | 0            |
| 8   | N     | 4     | 0        | 0        | 0       | 0            |
| 9   | B     | 7     | 0        | 0        | 0       | 0            |
| 9   | N     | 7     | 0        | 0        | 1       | 0            |
| 10  | B     | 8     | 0        | 0        | 0       | 0            |
| 10  | N     | 8     | 0        | 0        | 4       | 0            |
| 11  | A     | 53    | 0        | 31       | 8       | 0            |
| 11  | M     | 53    | 0        | 31       | 8       | 0            |
| 12  | C     | 19    | 0        | 20       | 3       | 0            |
| 12  | N     | 19    | 0        | 20       | 2       | 0            |
| 13  | O     | 111   | 0        | 174      | 0       | 0            |
| 13  | P     | 74    | 0        | 116      | 5       | 0            |
| 14  | A     | 16    | 0        | 20       | 5       | 0            |
| 15  | A     | 10    | 0        | 0        | 1       | 0            |
| 15  | B     | 1     | 0        | 0        | 0       | 0            |
| 15  | M     | 4     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 17071 | 0        | 16927    | 659     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (659) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:44:HIS:NE2   | 11:A:721:FAD:HM82 | 1.21        | 1.44     |
| 1:M:44:HIS:NE2   | 11:M:821:FAD:HM82 | 1.18        | 1.42     |
| 1:A:44:HIS:NE2   | 11:A:721:FAD:C8M  | 1.89        | 1.33     |
| 1:M:44:HIS:NE2   | 11:M:821:FAD:C8M  | 1.98        | 1.27     |
| 1:A:44:HIS:CE1   | 11:A:721:FAD:HM82 | 1.86        | 1.08     |
| 1:M:421:ASN:HD22 | 1:M:424:ALA:HB2   | 1.17        | 1.04     |
| 3:C:12:THR:HG22  | 3:C:14:THR:H      | 1.18        | 1.03     |
| 1:M:465:ILE:HD13 | 1:M:465:ILE:H     | 1.29        | 0.97     |
| 2:N:116:ILE:HG21 | 2:N:176:ALA:HB2   | 1.47        | 0.96     |
| 1:M:44:HIS:CE1   | 11:M:821:FAD:HM82 | 2.01        | 0.95     |
| 1:M:197:ARG:HD2  | 1:M:206:GLY:HA2   | 1.48        | 0.95     |
| 3:O:33:VAL:HB    | 3:O:34:PRO:HD3    | 1.52        | 0.92     |
| 2:N:189:LYS:HD3  | 2:N:189:LYS:H     | 1.34        | 0.91     |
| 1:M:469:PRO:HG3  | 1:M:534:ARG:HH21  | 1.36        | 0.90     |
| 3:O:75:THR:HG22  | 4:P:32:ILE:HD13   | 1.56        | 0.87     |
| 2:N:54:ARG:HE    | 2:N:103:VAL:HG13  | 1.39        | 0.87     |
| 1:M:304:ILE:HD12 | 1:M:304:ILE:H     | 1.40        | 0.86     |
| 2:N:15:PRO:HB2   | 3:O:5:LYS:H       | 1.41        | 0.85     |
| 1:M:316:LEU:HB3  | 1:M:319:LEU:HD12  | 1.59        | 0.85     |
| 1:M:447:ASN:HD21 | 1:M:449:ALA:HB3   | 1.42        | 0.84     |
| 1:M:7:LEU:HD21   | 1:M:411:THR:HA    | 1.60        | 0.84     |
| 1:M:421:ASN:HD22 | 1:M:424:ALA:CB    | 1.91        | 0.83     |
| 3:O:19:LEU:HD23  | 3:O:19:LEU:H      | 1.44        | 0.83     |
| 10:N:246:SF4:FE3 | 10:N:246:SF4:S2   | 1.69        | 0.83     |
| 1:A:413:ARG:HH11 | 1:A:413:ARG:HB2   | 1.43        | 0.82     |
| 3:C:104:GLY:HA2  | 3:C:107:PRO:HD2   | 1.62        | 0.82     |
| 3:O:31:THR:HG21  | 3:O:82:HIS:HB2    | 1.62        | 0.81     |
| 1:M:155:HIS:CD2  | 1:M:174:ASN:HA    | 2.15        | 0.81     |
| 1:M:549:LYS:HD2  | 1:M:565:TYR:HB3   | 1.62        | 0.81     |
| 3:O:126:VAL:HA   | 3:O:130:TRP:HB3   | 1.65        | 0.79     |
| 1:M:174:ASN:HD22 | 1:M:177:GLU:H     | 1.27        | 0.79     |
| 1:A:44:HIS:NE2   | 11:A:721:FAD:HM81 | 1.96        | 0.78     |
| 2:N:113:LEU:HD11 | 2:N:175:LEU:HD22  | 1.65        | 0.78     |
| 1:A:292:GLN:HE22 | 14:A:705:1PE:H261 | 1.51        | 0.75     |
| 1:M:236:LEU:HD22 | 1:M:339:VAL:HG11  | 1.67        | 0.75     |
| 2:N:116:ILE:HG21 | 2:N:176:ALA:CB    | 2.16        | 0.75     |
| 2:N:141:LYS:NZ   | 3:O:95:ASN:HB3    | 2.01        | 0.75     |
| 10:N:246:SF4:FE4 | 10:N:246:SF4:S1   | 1.77        | 0.75     |
| 4:P:51:TYR:HD1   | 4:P:52:GLU:HG3    | 1.49        | 0.75     |
| 2:N:206:PHE:HD1  | 12:N:800:HQO:H112 | 1.52        | 0.74     |
| 1:M:42:ARG:HH21  | 2:N:150:ASN:HB2   | 1.51        | 0.74     |
| 4:D:67:LEU:O     | 4:D:71:ILE:HG13   | 1.86        | 0.74     |
| 1:M:311:VAL:HG12 | 1:M:312:VAL:O     | 1.88        | 0.74     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:M:437:LYS:HG2   | 1:M:441:ASN:HD21  | 1.51        | 0.74     |
| 4:P:105:ALA:O     | 4:P:109:VAL:HG23  | 1.88        | 0.74     |
| 2:N:141:LYS:HZ1   | 3:O:95:ASN:HB3    | 1.53        | 0.73     |
| 1:M:465:ILE:N     | 1:M:465:ILE:HD13  | 2.03        | 0.73     |
| 1:M:152:PHE:HB3   | 1:M:155:HIS:ND1   | 2.02        | 0.73     |
| 2:B:225:GLN:HE22  | 12:C:700:HQO:H111 | 1.53        | 0.73     |
| 1:M:437:LYS:HG2   | 1:M:441:ASN:ND2   | 2.04        | 0.73     |
| 3:O:106:GLU:HB2   | 3:O:107:PRO:HD3   | 1.69        | 0.72     |
| 3:O:97:ILE:HD13   | 3:O:102:LYS:HA    | 1.70        | 0.72     |
| 1:M:488:ARG:HB3   | 1:M:488:ARG:NH1   | 2.04        | 0.72     |
| 1:M:251:GLY:HA2   | 1:M:277:PRO:HG2   | 1.70        | 0.72     |
| 1:M:88:HIS:O      | 1:M:401:VAL:HG22  | 1.89        | 0.72     |
| 13:P:810:CE1:H171 | 13:P:810:CE1:H211 | 1.72        | 0.72     |
| 2:N:11:VAL:HG21   | 2:N:91:GLU:HG2    | 1.70        | 0.72     |
| 4:P:104:ALA:O     | 4:P:108:THR:OG1   | 2.08        | 0.72     |
| 1:A:42:ARG:HG2    | 2:B:64:SER:HB3    | 1.71        | 0.71     |
| 1:A:184:ARG:HH11  | 1:A:184:ARG:HG2   | 1.54        | 0.71     |
| 3:C:19:LEU:HD12   | 3:C:20:PRO:HD2    | 1.72        | 0.71     |
| 3:C:12:THR:HG22   | 3:C:14:THR:N      | 2.02        | 0.71     |
| 3:O:50:LYS:HD2    | 4:P:117:THR:HG22  | 1.72        | 0.71     |
| 3:O:130:TRP:O     | 4:P:53:ARG:NH2    | 2.24        | 0.70     |
| 3:O:50:LYS:HD2    | 4:P:117:THR:CG2   | 2.21        | 0.70     |
| 4:P:60:SER:O      | 4:P:64:ARG:HG3    | 1.91        | 0.70     |
| 1:M:316:LEU:HD22  | 1:M:319:LEU:HD11  | 1.73        | 0.70     |
| 1:M:545:VAL:HG12  | 1:M:546:ASN:ND2   | 2.06        | 0.70     |
| 1:M:497:VAL:HG21  | 2:N:15:PRO:HG2    | 1.73        | 0.69     |
| 1:M:447:ASN:HD22  | 1:M:450:LYS:HG2   | 1.57        | 0.69     |
| 3:C:50:LYS:HB3    | 4:D:118:ILE:HG22  | 1.74        | 0.69     |
| 4:P:51:TYR:CD1    | 4:P:52:GLU:HG3    | 2.27        | 0.69     |
| 1:M:465:ILE:H     | 1:M:465:ILE:CD1   | 1.95        | 0.69     |
| 1:M:89:CYS:N      | 1:M:90:PRO:HD2    | 2.07        | 0.69     |
| 2:B:225:GLN:NE2   | 12:C:700:HQO:H111 | 2.07        | 0.69     |
| 1:A:413:ARG:HH11  | 1:A:413:ARG:CB    | 2.05        | 0.69     |
| 1:M:187:ALA:HB2   | 1:M:414:ALA:HB2   | 1.74        | 0.69     |
| 3:C:15:TRP:O      | 3:C:18:LYS:HG2    | 1.92        | 0.69     |
| 1:A:323:LYS:HG3   | 1:A:327:ARG:HH11  | 1.58        | 0.69     |
| 1:M:99:TRP:CD2    | 1:M:142:THR:HG21  | 2.27        | 0.69     |
| 1:A:484:GLU:HG3   | 1:A:488:ARG:NH1   | 2.08        | 0.69     |
| 3:O:120:THR:HG23  | 4:P:30:VAL:HB     | 1.76        | 0.68     |
| 1:A:390:ARG:HH22  | 6:A:702:OAA:C4    | 2.07        | 0.68     |
| 1:M:447:ASN:ND2   | 1:M:449:ALA:HB3   | 2.08        | 0.68     |
| 1:M:1:GLN:HG2     | 1:M:2:THR:H       | 1.57        | 0.68     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:549:LYS:HA   | 1:M:568:VAL:HG23 | 1.76        | 0.68     |
| 1:A:413:ARG:NH1  | 1:A:413:ARG:HB2  | 2.08        | 0.68     |
| 1:M:435:ARG:HA   | 1:M:438:ASP:OD2  | 1.94        | 0.68     |
| 1:M:421:ASN:ND2  | 1:M:424:ALA:HB2  | 2.01        | 0.67     |
| 1:M:342:ASP:HB3  | 1:M:345:LYS:HB3  | 1.77        | 0.67     |
| 1:A:484:GLU:HG3  | 1:A:488:ARG:HH12 | 1.60        | 0.67     |
| 2:B:222:ALA:HB2  | 3:C:92:LYS:HE3   | 1.77        | 0.67     |
| 3:C:33:VAL:HA    | 4:D:82:MET:CE    | 2.25        | 0.66     |
| 4:D:20:GLY:HA2   | 4:D:73:LEU:HB3   | 1.77        | 0.66     |
| 3:O:86:TRP:HE1   | 4:P:22:MET:CE    | 2.09        | 0.66     |
| 1:M:174:ASN:ND2  | 1:M:177:GLU:HG2  | 2.09        | 0.66     |
| 1:M:332:CYS:HA   | 1:M:343:PRO:HG2  | 1.78        | 0.66     |
| 4:P:48:ALA:HA    | 4:P:53:ARG:HD3   | 1.78        | 0.66     |
| 4:P:72:VAL:HG11  | 4:P:108:THR:HG23 | 1.77        | 0.66     |
| 3:C:50:LYS:HE2   | 3:C:50:LYS:HA    | 1.77        | 0.66     |
| 3:O:75:THR:HG22  | 4:P:32:ILE:CD1   | 2.25        | 0.66     |
| 4:P:7:ARG:HG2    | 4:P:8:SER:N      | 2.10        | 0.66     |
| 3:O:86:TRP:HE1   | 4:P:22:MET:HE2   | 1.62        | 0.65     |
| 1:M:84:TYR:HE2   | 1:M:405:LEU:HD22 | 1.61        | 0.65     |
| 2:N:196:ASN:ND2  | 2:N:234:ASP:OD1  | 2.30        | 0.65     |
| 3:C:33:VAL:HB    | 3:C:34:PRO:HD3   | 1.78        | 0.65     |
| 1:A:197:ARG:HD2  | 1:A:206:GLY:HA2  | 1.79        | 0.65     |
| 2:N:225:GLN:O    | 2:N:229:VAL:HG23 | 1.97        | 0.64     |
| 1:M:444:GLY:HA3  | 1:M:488:ARG:O    | 1.98        | 0.64     |
| 1:M:89:CYS:H     | 1:M:90:PRO:HD2   | 1.60        | 0.64     |
| 2:N:13:TYR:HB2   | 2:N:21:PRO:HB3   | 1.79        | 0.64     |
| 4:D:0:MET:HG2    | 4:D:1:ILE:H      | 1.63        | 0.64     |
| 1:A:27:ASN:ND2   | 1:A:30:ALA:HB2   | 2.12        | 0.64     |
| 4:P:77:CYS:O     | 4:P:81:ARG:HG3   | 1.97        | 0.64     |
| 1:A:324:LEU:CD1  | 1:A:344:VAL:HG22 | 2.28        | 0.64     |
| 1:M:391:LEU:O    | 1:M:394:ASN:HB2  | 1.98        | 0.63     |
| 1:M:217:LEU:HG   | 1:M:555:ARG:HB3  | 1.78        | 0.63     |
| 1:M:275:GLY:O    | 1:M:277:PRO:HD3  | 1.99        | 0.63     |
| 3:O:60:VAL:O     | 3:O:64:GLN:HG3   | 1.99        | 0.63     |
| 1:M:251:GLY:HA2  | 1:M:277:PRO:CG   | 2.28        | 0.63     |
| 1:M:435:ARG:HH12 | 1:M:439:LEU:HD22 | 1.64        | 0.63     |
| 2:B:16:GLU:OE2   | 3:C:3:LYS:HD2    | 1.98        | 0.63     |
| 1:M:327:ARG:O    | 1:M:328:LEU:HD23 | 1.98        | 0.63     |
| 2:N:57:CYS:HB3   | 2:N:62:CYS:HB3   | 1.79        | 0.63     |
| 1:A:279:ASN:O    | 1:A:280:LYS:HB2  | 1.99        | 0.62     |
| 4:P:24:SER:O     | 4:P:28:ALA:HB3   | 1.99        | 0.62     |
| 1:M:436:LEU:O    | 1:M:440:VAL:HG23 | 1.99        | 0.62     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:N:135:THR:HG23 | 2:N:136:PRO:HD2   | 1.82        | 0.62     |
| 1:M:202:ASN:HA   | 1:M:353:THR:HG22  | 1.82        | 0.62     |
| 2:N:206:PHE:CE1  | 2:N:225:GLN:HG3   | 2.35        | 0.62     |
| 1:M:41:MET:HB2   | 1:M:137:HIS:CE1   | 2.34        | 0.62     |
| 1:M:199:TYR:CE1  | 1:M:229:VAL:HG11  | 2.35        | 0.61     |
| 1:M:51:GLY:HA2   | 1:M:131:THR:HG21  | 1.82        | 0.61     |
| 1:M:332:CYS:O    | 1:M:336:LYS:HG3   | 2.00        | 0.61     |
| 3:C:130:TRP:CD1  | 3:C:130:TRP:N     | 2.69        | 0.61     |
| 4:D:48:ALA:O     | 4:D:53:ARG:HD3    | 2.00        | 0.61     |
| 1:M:444:GLY:HA3  | 1:M:488:ARG:C     | 2.21        | 0.61     |
| 4:D:13:PHE:HE2   | 4:D:97:LYS:HE2    | 1.65        | 0.61     |
| 3:O:18:LYS:HD2   | 3:O:19:LEU:HD22   | 1.81        | 0.61     |
| 1:A:336:LYS:O    | 1:A:340:GLY:HA2   | 2.00        | 0.60     |
| 4:P:22:MET:O     | 4:P:26:ILE:HD13   | 2.01        | 0.60     |
| 3:C:33:VAL:HA    | 4:D:82:MET:HE3    | 1.83        | 0.60     |
| 2:N:236:LEU:HD23 | 2:N:236:LEU:C     | 2.22        | 0.60     |
| 2:N:206:PHE:CD1  | 12:N:800:HQO:H112 | 2.33        | 0.60     |
| 1:M:11:GLY:O     | 1:M:16:GLY:HA3    | 2.01        | 0.60     |
| 1:M:192:THR:OG1  | 1:M:212:GLY:HA3   | 2.02        | 0.60     |
| 1:M:82:VAL:HG22  | 1:M:385:LEU:HD12  | 1.82        | 0.60     |
| 1:A:358:MET:HE3  | 1:A:389:ASN:HA    | 1.83        | 0.60     |
| 4:D:63:GLY:O     | 4:D:67:LEU:HD23   | 2.02        | 0.59     |
| 1:A:94:THR:HG23  | 2:B:131:THR:HG22  | 1.83        | 0.59     |
| 4:D:86:MET:HA    | 4:D:86:MET:HE3    | 1.83        | 0.59     |
| 1:M:92:GLU:HB3   | 1:M:400:VAL:HB    | 1.83        | 0.59     |
| 1:M:195:ALA:O    | 1:M:198:VAL:HG22  | 2.02        | 0.59     |
| 1:M:156:PHE:CD2  | 1:M:503:LEU:HD22  | 2.37        | 0.59     |
| 1:A:28:PRO:HA    | 1:A:148:GLN:HE21  | 1.65        | 0.59     |
| 1:A:148:GLN:N    | 1:A:148:GLN:OE1   | 2.30        | 0.59     |
| 1:M:96:LEU:HD21  | 1:M:139:LEU:HD21  | 1.85        | 0.59     |
| 3:O:50:LYS:HG3   | 4:P:118:ILE:HA    | 1.84        | 0.59     |
| 1:A:343:PRO:HG3  | 1:A:348:ILE:HD11  | 1.85        | 0.59     |
| 1:A:372:LYS:HE3  | 1:A:413:ARG:HE    | 1.67        | 0.59     |
| 4:D:78:GLY:O     | 4:D:82:MET:HG3    | 2.03        | 0.59     |
| 1:M:84:TYR:CE2   | 1:M:405:LEU:HD22  | 2.38        | 0.59     |
| 2:B:57:CYS:O     | 2:B:58:ARG:HB2    | 2.02        | 0.59     |
| 1:A:289:LYS:NZ   | 14:A:705:1PE:H262 | 2.18        | 0.59     |
| 2:N:44:LYS:HD3   | 2:N:51:LEU:O      | 2.03        | 0.58     |
| 1:A:232:HIS:HD2  | 1:A:234:THR:H     | 1.50        | 0.58     |
| 1:M:44:HIS:CE1   | 1:M:204:ASN:HA    | 2.38        | 0.58     |
| 2:N:116:ILE:HG22 | 2:N:191:ARG:HD3   | 1.86        | 0.58     |
| 1:A:358:MET:CE   | 1:A:389:ASN:HA    | 2.33        | 0.58     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:200:ARG:NH1  | 1:A:201:TYR:OH    | 2.37        | 0.58     |
| 1:M:181:VAL:HG12 | 1:M:182:GLN:H     | 1.67        | 0.58     |
| 1:M:331:ILE:H    | 1:M:331:ILE:HD12  | 1.69        | 0.58     |
| 2:B:241:LYS:O    | 2:B:241:LYS:HG3   | 2.02        | 0.58     |
| 1:A:103:TRP:O    | 2:B:139:MET:HE1   | 2.04        | 0.58     |
| 2:N:157:ALA:HB1  | 2:N:209:TYR:CD2   | 2.38        | 0.58     |
| 1:A:390:ARG:HD2  | 1:A:395:SER:HB2   | 1.86        | 0.58     |
| 3:O:36:VAL:HG11  | 4:P:82:MET:HE1    | 1.85        | 0.58     |
| 2:N:54:ARG:NE    | 2:N:103:VAL:HG13  | 2.13        | 0.58     |
| 3:O:106:GLU:H    | 3:O:106:GLU:CD    | 2.08        | 0.58     |
| 3:O:36:VAL:HG11  | 4:P:82:MET:CE     | 2.33        | 0.57     |
| 3:O:98:VAL:HG23  | 3:O:103:MET:HB2   | 1.85        | 0.57     |
| 1:M:499:ASN:C    | 1:M:499:ASN:HD22  | 2.06        | 0.57     |
| 1:M:448:TRP:CH2  | 1:M:504:TYR:HB3   | 2.38        | 0.57     |
| 1:A:556:ASP:HB2  | 1:A:558:ASP:OD2   | 2.04        | 0.57     |
| 1:M:341:VAL:HG13 | 1:M:346:GLU:HB2   | 1.86        | 0.57     |
| 4:P:9:ASP:C      | 4:P:11:PRO:HD2    | 2.24        | 0.57     |
| 4:P:64:ARG:HB3   | 4:P:115:VAL:HG22  | 1.87        | 0.57     |
| 1:A:366:ASN:HB3  | 1:A:409:GLN:HG3   | 1.84        | 0.57     |
| 1:M:181:VAL:HG12 | 1:M:182:GLN:N     | 2.19        | 0.57     |
| 2:B:157:ALA:HB1  | 2:B:209:TYR:CD2   | 2.39        | 0.57     |
| 1:A:324:LEU:HD12 | 1:A:344:VAL:HG22  | 1.86        | 0.57     |
| 2:N:11:VAL:CG2   | 2:N:91:GLU:HG2    | 2.34        | 0.57     |
| 1:M:209:THR:O    | 1:M:209:THR:HG22  | 2.04        | 0.57     |
| 2:B:206:PHE:HD1  | 12:C:700:HQO:H112 | 1.69        | 0.56     |
| 1:A:462:GLY:HA3  | 1:A:475:THR:OG1   | 2.05        | 0.56     |
| 4:D:68:PHE:HD1   | 4:D:111:THR:HG22  | 1.70        | 0.56     |
| 2:N:2:GLU:OE1    | 2:N:2:GLU:HA      | 2.04        | 0.56     |
| 1:M:304:ILE:HG12 | 1:M:313:TYR:HE2   | 1.71        | 0.56     |
| 1:A:18:ARG:HG2   | 1:A:400:VAL:HA    | 1.88        | 0.56     |
| 4:P:76:TRP:NE1   | 13:P:810:CE1:H362 | 2.21        | 0.56     |
| 3:C:33:VAL:HG22  | 4:D:82:MET:CE     | 2.36        | 0.56     |
| 1:M:510:HIS:O    | 1:M:514:VAL:HG23  | 2.06        | 0.56     |
| 4:D:83:HIS:O     | 4:D:86:MET:HB2    | 2.06        | 0.56     |
| 2:B:188:LYS:NZ   | 2:B:230:GLU:HG3   | 2.20        | 0.56     |
| 1:M:358:MET:SD   | 1:M:390:ARG:N     | 2.79        | 0.56     |
| 3:O:104:GLY:O    | 3:O:107:PRO:HD2   | 2.06        | 0.55     |
| 1:M:545:VAL:C    | 1:M:546:ASN:HD22  | 2.08        | 0.55     |
| 2:N:135:THR:HG22 | 2:N:137:ALA:H     | 1.71        | 0.55     |
| 1:A:321:GLU:HA   | 1:A:321:GLU:OE1   | 2.06        | 0.55     |
| 1:M:102:PRO:HB2  | 2:N:139:MET:CE    | 2.36        | 0.55     |
| 1:M:152:PHE:O    | 1:M:155:HIS:HB2   | 2.06        | 0.55     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:P:112:LEU:O    | 4:P:116:VAL:HG22 | 2.07        | 0.55     |
| 1:M:260:TYR:CE1  | 1:M:264:GLN:NE2  | 2.75        | 0.55     |
| 3:O:19:LEU:HD21  | 3:O:22:TYR:CE2   | 2.41        | 0.55     |
| 3:C:50:LYS:HD3   | 4:D:118:ILE:HG22 | 1.88        | 0.55     |
| 1:M:435:ARG:O    | 1:M:438:ASP:HB2  | 2.07        | 0.55     |
| 1:M:311:VAL:HG11 | 1:M:349:PRO:HB2  | 1.89        | 0.55     |
| 1:M:323:LYS:HG2  | 1:M:327:ARG:HH21 | 1.71        | 0.55     |
| 4:D:112:LEU:O    | 4:D:116:VAL:HG22 | 2.06        | 0.55     |
| 1:A:250:GLU:HB3  | 1:A:319:LEU:HD11 | 1.89        | 0.55     |
| 3:O:19:LEU:H     | 3:O:19:LEU:CD2   | 2.19        | 0.55     |
| 2:N:201:VAL:HG23 | 2:N:202:TRP:N    | 2.21        | 0.55     |
| 2:N:21:PRO:HD2   | 3:O:7:TYR:CE2    | 2.42        | 0.55     |
| 3:C:106:GLU:CD   | 3:C:106:GLU:H    | 2.10        | 0.55     |
| 1:M:62:PHE:HB3   | 1:M:86:VAL:HG23  | 1.89        | 0.55     |
| 2:B:2:GLU:HA     | 2:B:2:GLU:OE2    | 2.06        | 0.55     |
| 2:B:8:ILE:HD11   | 2:B:81:LEU:HD11  | 1.89        | 0.55     |
| 2:N:202:TRP:CZ2  | 4:P:11:PRO:HG3   | 2.42        | 0.54     |
| 1:A:182:GLN:OE1  | 1:A:184:ARG:NH1  | 2.33        | 0.54     |
| 1:A:323:LYS:HG3  | 1:A:327:ARG:NH1  | 2.22        | 0.54     |
| 1:M:162:VAL:HG22 | 1:M:167:VAL:HA   | 1.89        | 0.54     |
| 1:A:527:GLU:OE1  | 1:A:529:ARG:HD2  | 2.07        | 0.54     |
| 2:B:155:TYR:CE2  | 2:B:169:GLY:HA3  | 2.43        | 0.54     |
| 1:M:219:HIS:O    | 1:M:371:ILE:HD11 | 2.07        | 0.54     |
| 3:O:70:ILE:O     | 3:O:73:LEU:HB2   | 2.07        | 0.54     |
| 1:M:168:ARG:HD3  | 1:M:425:ILE:CD1  | 2.37        | 0.54     |
| 4:P:72:VAL:CG1   | 4:P:108:THR:HG23 | 2.38        | 0.54     |
| 3:C:50:LYS:HB3   | 4:D:118:ILE:CG2  | 2.36        | 0.54     |
| 2:B:32:ALA:O     | 2:B:82:ARG:NH1   | 2.40        | 0.54     |
| 1:M:242:LEU:HD12 | 1:M:243:MET:N    | 2.22        | 0.54     |
| 1:M:253:ILE:HA   | 1:M:283:GLU:HG2  | 1.90        | 0.54     |
| 1:A:341:VAL:HG13 | 1:A:346:GLU:HB2  | 1.88        | 0.54     |
| 2:N:81:LEU:HD12  | 2:N:81:LEU:N     | 2.22        | 0.54     |
| 2:B:57:CYS:HB3   | 2:B:62:CYS:HB3   | 1.90        | 0.54     |
| 1:M:551:THR:HG23 | 1:M:563:LEU:HD22 | 1.90        | 0.54     |
| 4:P:3:PRO:O      | 4:P:4:ASN:C      | 2.46        | 0.54     |
| 1:M:308:ARG:NH1  | 1:M:339:VAL:HG12 | 2.23        | 0.54     |
| 1:A:7:LEU:HD21   | 1:A:32:ILE:HG12  | 1.90        | 0.54     |
| 1:M:95:GLN:OE1   | 1:M:98:LEU:HD12  | 2.07        | 0.54     |
| 1:M:217:LEU:HG   | 1:M:555:ARG:CB   | 2.39        | 0.53     |
| 1:A:184:ARG:NH1  | 1:A:184:ARG:HG2  | 2.22        | 0.53     |
| 1:M:331:ILE:N    | 1:M:331:ILE:HD12 | 2.23        | 0.53     |
| 1:A:11:GLY:O     | 1:A:16:GLY:HA3   | 2.08        | 0.53     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:M:76:LEU:HD12  | 1:M:388:ALA:HB2   | 1.90        | 0.53     |
| 2:N:134:GLN:NE2  | 2:N:184:ARG:HD3   | 2.23        | 0.53     |
| 4:P:117:THR:O    | 4:P:118:ILE:C     | 2.46        | 0.53     |
| 4:P:73:LEU:HB2   | 4:P:74:PRO:HD3    | 1.90        | 0.53     |
| 1:M:311:VAL:HG11 | 1:M:349:PRO:CB    | 2.39        | 0.53     |
| 4:D:98:TRP:NE1   | 13:P:810:CE1:H141 | 2.24        | 0.53     |
| 3:C:98:VAL:HG23  | 3:C:98:VAL:O      | 2.08        | 0.53     |
| 1:M:147:PRO:HD2  | 1:M:148:GLN:OE1   | 2.09        | 0.53     |
| 1:A:200:ARG:HG3  | 1:A:457:LEU:HD23  | 1.91        | 0.53     |
| 1:A:192:THR:OG1  | 1:A:212:GLY:HA3   | 2.08        | 0.53     |
| 1:M:7:LEU:HD12   | 1:M:23:ALA:HB1    | 1.91        | 0.53     |
| 4:P:102:GLY:HA2  | 13:P:710:CE1:H42  | 1.91        | 0.53     |
| 1:M:425:ILE:O    | 1:M:428:GLN:HB2   | 2.09        | 0.52     |
| 1:M:545:VAL:HG12 | 1:M:546:ASN:HD22  | 1.74        | 0.52     |
| 1:M:168:ARG:HD3  | 1:M:425:ILE:HD11  | 1.91        | 0.52     |
| 1:M:81:VAL:HG21  | 1:M:383:VAL:O     | 2.09        | 0.52     |
| 1:M:331:ILE:H    | 1:M:331:ILE:CD1   | 2.23        | 0.52     |
| 1:M:151:ARG:NH1  | 1:M:153:ASP:OD2   | 2.43        | 0.52     |
| 2:N:9:GLU:HG3    | 2:N:25:PHE:CZ     | 2.44        | 0.52     |
| 4:P:39:LEU:HD13  | 4:P:49:LEU:HB3    | 1.90        | 0.52     |
| 1:A:90:PRO:HB2   | 15:A:758:HOH:O    | 2.09        | 0.52     |
| 1:M:242:LEU:HD23 | 11:M:821:FAD:HM73 | 1.91        | 0.52     |
| 4:P:10:GLU:N     | 4:P:11:PRO:CD     | 2.73        | 0.52     |
| 1:A:436:LEU:O    | 1:A:440:VAL:HG23  | 2.10        | 0.52     |
| 2:B:242:PRO:HG3  | 4:P:94:PRO:HD3    | 1.89        | 0.52     |
| 1:M:58:ASP:C     | 1:M:60:ASP:H      | 2.11        | 0.52     |
| 1:A:118:GLY:HA2  | 1:A:279:ASN:HD21  | 1.73        | 0.52     |
| 4:D:13:PHE:CE2   | 4:D:97:LYS:HE2    | 2.45        | 0.52     |
| 2:N:139:MET:HA   | 2:N:142:TYR:CE2   | 2.45        | 0.52     |
| 1:A:292:GLN:NE2  | 14:A:705:1PE:H261 | 2.21        | 0.52     |
| 3:C:50:LYS:CB    | 4:D:118:ILE:HG22  | 2.40        | 0.52     |
| 2:B:229:VAL:HG12 | 2:B:233:LYS:HE3   | 1.92        | 0.52     |
| 2:N:169:GLY:O    | 2:N:173:ILE:HG13  | 2.10        | 0.52     |
| 1:A:232:HIS:CE1  | 1:A:242:LEU:HD11  | 2.45        | 0.52     |
| 2:N:97:PRO:HG2   | 2:N:105:ASP:HB3   | 1.92        | 0.52     |
| 2:N:233:LYS:O    | 2:N:237:ILE:HD13  | 2.10        | 0.52     |
| 1:M:10:VAL:HG13  | 1:M:157:VAL:HG21  | 1.91        | 0.52     |
| 1:M:122:GLU:H    | 1:M:122:GLU:CD    | 2.13        | 0.52     |
| 3:C:113:TRP:O    | 3:C:117:VAL:HG23  | 2.09        | 0.52     |
| 1:M:7:LEU:HD11   | 1:M:411:THR:OG1   | 2.10        | 0.51     |
| 1:M:328:LEU:N    | 1:M:329:PRO:HD3   | 2.24        | 0.51     |
| 1:A:356:TYR:CE2  | 1:A:390:ARG:HD3   | 2.45        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:N:28:VAL:HG22  | 2:N:43:ILE:HD11  | 1.92        | 0.51     |
| 1:M:467:ARG:NH1  | 1:M:532:HIS:ND1  | 2.58        | 0.51     |
| 1:M:546:ASN:N    | 1:M:546:ASN:HD22 | 2.06        | 0.51     |
| 1:M:227:GLU:HB2  | 1:M:522:ALA:HB2  | 1.93        | 0.51     |
| 2:B:212:GLU:HG3  | 3:C:21:PHE:CE2   | 2.45        | 0.51     |
| 2:N:113:LEU:CD1  | 2:N:175:LEU:HD22 | 2.39        | 0.51     |
| 1:M:328:LEU:N    | 1:M:329:PRO:CD   | 2.74        | 0.51     |
| 1:M:98:LEU:HD11  | 2:N:127:ALA:HA   | 1.92        | 0.51     |
| 3:C:59:PHE:CE1   | 3:C:63:LEU:HD11  | 2.46        | 0.51     |
| 4:D:93:VAL:N     | 2:N:243:ARG:O    | 2.42        | 0.51     |
| 2:N:28:VAL:CG2   | 2:N:43:ILE:HD11  | 2.41        | 0.51     |
| 1:M:171:VAL:HG11 | 1:M:432:VAL:HG11 | 1.93        | 0.51     |
| 2:N:198:GLN:O    | 2:N:203:SER:HB2  | 2.10        | 0.51     |
| 3:C:50:LYS:CG    | 4:D:118:ILE:HG22 | 2.41        | 0.50     |
| 4:D:73:LEU:HB2   | 4:D:74:PRO:HD3   | 1.93        | 0.50     |
| 3:O:33:VAL:O     | 3:O:36:VAL:HG22  | 2.11        | 0.50     |
| 1:M:308:ARG:HH12 | 1:M:339:VAL:HG12 | 1.76        | 0.50     |
| 1:M:145:GLN:O    | 1:M:147:PRO:HD3  | 2.12        | 0.50     |
| 1:M:296:HIS:ND1  | 1:M:299:ARG:NH2  | 2.59        | 0.50     |
| 1:M:21:ILE:HG21  | 1:M:99:TRP:CH2   | 2.47        | 0.50     |
| 1:M:0:MET:SD     | 1:M:182:GLN:HB2  | 2.51        | 0.50     |
| 1:M:158:LEU:HD11 | 1:M:436:LEU:HD22 | 1.93        | 0.50     |
| 1:M:413:ARG:HB2  | 1:M:413:ARG:NH1  | 2.26        | 0.50     |
| 1:M:311:VAL:HG13 | 1:M:350:VAL:O    | 2.11        | 0.50     |
| 2:N:241:LYS:O    | 2:N:243:ARG:HG3  | 2.12        | 0.50     |
| 1:M:39:TYR:HE2   | 2:N:54:ARG:HH12  | 1.59        | 0.50     |
| 1:M:174:ASN:ND2  | 1:M:177:GLU:H    | 2.03        | 0.50     |
| 1:A:42:ARG:CG    | 2:B:64:SER:HB3   | 2.42        | 0.50     |
| 2:B:234:ASP:OD1  | 4:D:7:ARG:NH2    | 2.44        | 0.50     |
| 3:C:50:LYS:HD2   | 4:D:118:ILE:O    | 2.11        | 0.50     |
| 1:M:171:VAL:HB   | 1:M:432:VAL:HG11 | 1.94        | 0.50     |
| 1:M:435:ARG:NH1  | 1:M:439:LEU:HB2  | 2.27        | 0.50     |
| 1:M:75:TRP:O     | 1:M:568:VAL:HG11 | 2.12        | 0.49     |
| 4:P:118:ILE:OXT  | 4:P:118:ILE:HG23 | 2.11        | 0.49     |
| 1:M:330:PHE:HB3  | 1:M:331:ILE:HD12 | 1.94        | 0.49     |
| 1:A:316:LEU:O    | 1:A:319:LEU:HB2  | 2.10        | 0.49     |
| 1:M:162:VAL:HG13 | 1:M:166:HIS:O    | 2.12        | 0.49     |
| 3:O:118:VAL:O    | 3:O:122:VAL:HG23 | 2.12        | 0.49     |
| 3:C:127:ALA:O    | 3:C:128:LEU:HD23 | 2.12        | 0.49     |
| 1:M:196:GLY:HA3  | 1:M:204:ASN:OD1  | 2.13        | 0.49     |
| 1:M:316:LEU:HB3  | 1:M:319:LEU:CD1  | 2.35        | 0.49     |
| 1:M:42:ARG:HD2   | 2:N:64:SER:OG    | 2.13        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:66:PHE:HD1   | 1:M:82:VAL:HG12  | 1.78        | 0.49     |
| 1:A:159:ASP:OD2  | 1:A:160:ILE:N    | 2.46        | 0.49     |
| 2:N:92:ALA:HB1   | 2:N:104:VAL:CG1  | 2.42        | 0.49     |
| 3:O:33:VAL:HB    | 3:O:34:PRO:CD    | 2.34        | 0.49     |
| 2:N:189:LYS:CD   | 2:N:189:LYS:H    | 2.12        | 0.49     |
| 2:N:96:PHE:HB3   | 2:N:104:VAL:HB   | 1.94        | 0.49     |
| 3:C:33:VAL:HG22  | 4:D:82:MET:HE2   | 1.92        | 0.49     |
| 1:M:102:PRO:HB2  | 2:N:139:MET:HE1  | 1.95        | 0.49     |
| 1:M:304:ILE:HD12 | 1:M:304:ILE:N    | 2.18        | 0.49     |
| 1:M:187:ALA:CB   | 1:M:414:ALA:HB2  | 2.41        | 0.49     |
| 4:P:28:ALA:N     | 4:P:29:PRO:HD2   | 2.28        | 0.49     |
| 2:N:180:ASN:OD1  | 2:N:188:LYS:HA   | 2.12        | 0.49     |
| 4:D:10:GLU:N     | 4:D:11:PRO:HD2   | 2.27        | 0.49     |
| 1:M:488:ARG:HB3  | 1:M:488:ARG:HH11 | 1.75        | 0.49     |
| 1:M:141:GLN:HB3  | 2:N:118:PRO:O    | 2.13        | 0.49     |
| 1:M:155:HIS:HD2  | 1:M:174:ASN:HA   | 1.74        | 0.49     |
| 1:M:100:GLY:O    | 1:M:101:CYS:C    | 2.52        | 0.49     |
| 1:A:549:LYS:HD2  | 1:A:565:TYR:HB3  | 1.95        | 0.49     |
| 1:M:104:SER:O    | 1:M:105:ARG:HD3  | 2.12        | 0.49     |
| 4:P:55:LEU:CD1   | 4:P:118:ILE:HD11 | 2.43        | 0.49     |
| 1:A:317:ARG:C    | 1:A:319:LEU:H    | 2.17        | 0.49     |
| 1:M:171:VAL:CG1  | 1:M:432:VAL:HG11 | 2.42        | 0.49     |
| 3:O:127:ALA:O    | 3:O:128:LEU:HD23 | 2.13        | 0.49     |
| 3:O:90:ALA:N     | 3:O:91:PRO:HD2   | 2.28        | 0.49     |
| 2:N:159:PRO:HG2  | 2:N:207:VAL:HG21 | 1.94        | 0.49     |
| 1:M:549:LYS:HD2  | 1:M:565:TYR:CB   | 2.39        | 0.48     |
| 1:M:435:ARG:HH12 | 1:M:439:LEU:CD2  | 2.25        | 0.48     |
| 2:N:201:VAL:CG2  | 2:N:202:TRP:N    | 2.76        | 0.48     |
| 1:M:236:LEU:HD22 | 1:M:339:VAL:CG1  | 2.41        | 0.48     |
| 1:A:115:ARG:HD3  | 1:A:279:ASN:ND2  | 2.28        | 0.48     |
| 1:M:213:MET:CE   | 1:M:380:CYS:HA   | 2.43        | 0.48     |
| 1:M:304:ILE:HG22 | 1:M:305:SER:N    | 2.28        | 0.48     |
| 1:A:109:GLY:HA2  | 2:B:134:GLN:O    | 2.13        | 0.48     |
| 4:P:86:MET:HE3   | 4:P:91:ILE:HB    | 1.95        | 0.48     |
| 1:A:44:HIS:NE2   | 11:A:721:FAD:C8  | 2.73        | 0.48     |
| 2:B:201:VAL:HG23 | 2:B:202:TRP:N    | 2.28        | 0.48     |
| 2:N:175:LEU:O    | 2:N:178:ARG:HB3  | 2.13        | 0.48     |
| 1:M:62:PHE:CD2   | 1:M:87:HIS:HA    | 2.49        | 0.48     |
| 1:A:196:GLY:HA3  | 1:A:204:ASN:OD1  | 2.14        | 0.48     |
| 1:A:448:TRP:CH2  | 1:A:504:TYR:HB3  | 2.49        | 0.48     |
| 1:A:556:ASP:OD2  | 1:A:562:ARG:NE   | 2.43        | 0.48     |
| 4:D:93:VAL:HA    | 4:D:94:PRO:HD2   | 1.73        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:1:GLN:HG2    | 1:M:2:THR:N      | 2.27        | 0.48     |
| 4:P:70:MET:O     | 4:P:74:PRO:HG2   | 2.13        | 0.48     |
| 4:P:39:LEU:HB2   | 4:P:49:LEU:HD13  | 1.96        | 0.48     |
| 1:A:85:PHE:CD2   | 1:A:385:LEU:HD11 | 2.49        | 0.48     |
| 1:M:469:PRO:HG3  | 1:M:534:ARG:NH2  | 2.16        | 0.48     |
| 1:M:159:ASP:OD2  | 1:M:160:ILE:N    | 2.47        | 0.48     |
| 3:C:75:THR:HG22  | 4:D:32:ILE:HD13  | 1.96        | 0.48     |
| 1:M:35:ILE:CD1   | 1:M:155:HIS:HB3  | 2.44        | 0.48     |
| 3:O:91:PRO:C     | 3:O:93:ALA:H     | 2.16        | 0.48     |
| 2:N:54:ARG:O     | 2:N:55:TRP:HB3   | 2.15        | 0.47     |
| 1:M:63:GLU:O     | 1:M:66:PHE:HB3   | 2.14        | 0.47     |
| 1:M:130:LYS:O    | 1:M:133:PHE:HB3  | 2.14        | 0.47     |
| 1:M:165:GLY:O    | 1:M:372:LYS:HB2  | 2.13        | 0.47     |
| 1:M:382:SER:C    | 1:M:384:GLY:H    | 2.17        | 0.47     |
| 2:N:81:LEU:H     | 2:N:81:LEU:CD1   | 2.27        | 0.47     |
| 1:A:439:LEU:HD12 | 1:A:442:GLN:NE2  | 2.29        | 0.47     |
| 1:A:224:ARG:NH2  | 1:A:382:SER:O    | 2.41        | 0.47     |
| 2:B:149:ILE:HG13 | 2:B:151:CYS:HB3  | 1.96        | 0.47     |
| 1:M:184:ARG:NH2  | 1:M:426:GLU:HG2  | 2.29        | 0.47     |
| 1:M:311:VAL:HG12 | 1:M:312:VAL:N    | 2.30        | 0.47     |
| 1:M:66:PHE:CD1   | 1:M:82:VAL:HG12  | 2.50        | 0.47     |
| 1:M:499:ASN:HD21 | 1:M:501:ASP:HB3  | 1.79        | 0.47     |
| 1:M:286:PRO:O    | 1:M:290:VAL:HG23 | 2.15        | 0.47     |
| 2:N:194:GLN:HE22 | 4:P:1:ILE:HG21   | 1.79        | 0.47     |
| 2:B:28:VAL:HG12  | 2:B:29:PRO:O     | 2.14        | 0.47     |
| 2:B:113:LEU:HD23 | 2:B:113:LEU:O    | 2.13        | 0.47     |
| 2:N:135:THR:CG2  | 2:N:136:PRO:HD2  | 2.45        | 0.47     |
| 1:A:377:VAL:HG21 | 1:A:403:GLY:HA2  | 1.97        | 0.47     |
| 1:M:493:ASP:OD1  | 2:N:50:ASP:HB3   | 2.15        | 0.47     |
| 2:B:195:LEU:O    | 2:B:201:VAL:HG22 | 2.15        | 0.47     |
| 1:M:479:LEU:HB3  | 1:M:516:GLU:HG2  | 1.97        | 0.47     |
| 3:C:31:THR:O     | 3:C:34:PRO:HD2   | 2.15        | 0.47     |
| 1:A:89:CYS:HB2   | 1:A:90:PRO:HD3   | 1.96        | 0.47     |
| 3:O:39:SER:OG    | 4:P:71:ILE:O     | 2.33        | 0.47     |
| 3:C:53:PRO:HD3   | 4:D:51:TYR:CZ    | 2.50        | 0.47     |
| 2:B:135:THR:O    | 2:B:136:PRO:C    | 2.52        | 0.47     |
| 4:P:79:LEU:HD23  | 4:P:82:MET:CE    | 2.45        | 0.46     |
| 3:C:50:LYS:CD    | 4:D:118:ILE:HG22 | 2.46        | 0.46     |
| 1:A:151:ARG:NH2  | 2:B:114:GLU:OE2  | 2.48        | 0.46     |
| 4:P:10:GLU:N     | 4:P:11:PRO:HD2   | 2.30        | 0.46     |
| 1:A:244:THR:H    | 1:A:331:ILE:HD11 | 1.79        | 0.46     |
| 1:M:232:HIS:O    | 1:M:352:PRO:HA   | 2.15        | 0.46     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:N:160:GLN:NE2  | 2:N:205:THR:OG1   | 2.47        | 0.46     |
| 1:A:232:HIS:NE2  | 1:A:242:LEU:HD11  | 2.30        | 0.46     |
| 1:M:393:SER:HA   | 11:M:821:FAD:O2   | 2.15        | 0.46     |
| 1:A:287:ARG:H    | 14:A:705:1PE:H122 | 1.81        | 0.46     |
| 1:M:247:CYS:CB   | 1:M:314:LEU:HD21  | 2.46        | 0.46     |
| 1:A:184:ARG:CG   | 1:A:184:ARG:NH1   | 2.78        | 0.46     |
| 2:B:188:LYS:HZ1  | 2:B:230:GLU:HG3   | 1.81        | 0.46     |
| 1:M:479:LEU:O    | 1:M:483:GLN:HG2   | 2.16        | 0.46     |
| 4:D:64:ARG:NH1   | 4:D:117:THR:HG23  | 2.30        | 0.46     |
| 4:P:39:LEU:N     | 4:P:40:PRO:HD2    | 2.30        | 0.46     |
| 1:A:244:THR:HG22 | 1:A:331:ILE:HG13  | 1.97        | 0.46     |
| 1:A:142:THR:O    | 1:A:145:GLN:HG2   | 2.15        | 0.46     |
| 2:N:145:PHE:HA   | 2:N:218:VAL:HG13  | 1.97        | 0.46     |
| 2:N:133:ILE:HG22 | 2:N:133:ILE:O     | 2.14        | 0.46     |
| 2:N:214:CYS:SG   | 10:N:246:SF4:S1   | 3.14        | 0.46     |
| 4:P:109:VAL:O    | 4:P:112:LEU:HB3   | 2.16        | 0.46     |
| 1:M:364:ASP:CG   | 1:M:366:ASN:H     | 2.19        | 0.46     |
| 2:N:15:PRO:CB    | 3:O:5:LYS:H       | 2.18        | 0.46     |
| 1:M:40:PRO:HB2   | 1:M:140:PHE:CD1   | 2.51        | 0.46     |
| 1:M:174:ASN:ND2  | 1:M:177:GLU:CG    | 2.77        | 0.46     |
| 2:N:158:CYS:HA   | 2:N:159:PRO:HD3   | 1.85        | 0.46     |
| 1:M:304:ILE:H    | 1:M:304:ILE:CD1   | 2.16        | 0.45     |
| 1:M:263:LEU:CD1  | 1:M:283:GLU:HA    | 2.45        | 0.45     |
| 2:N:81:LEU:H     | 2:N:81:LEU:HD12   | 1.81        | 0.45     |
| 2:N:167:PHE:CD1  | 2:N:203:SER:HB3   | 2.51        | 0.45     |
| 1:M:448:TRP:CG   | 1:M:449:ALA:N     | 2.84        | 0.45     |
| 1:A:206:GLY:HA3  | 2:B:55:TRP:CH2    | 2.51        | 0.45     |
| 2:N:41:GLY:CA    | 7:N:803:ACT:H2    | 2.46        | 0.45     |
| 1:M:315:ASP:OD1  | 1:M:317:ARG:HG3   | 2.15        | 0.45     |
| 1:A:40:PRO:HB2   | 1:A:140:PHE:CD1   | 2.51        | 0.45     |
| 4:P:93:VAL:HA    | 4:P:94:PRO:HD2    | 1.78        | 0.45     |
| 1:A:546:ASN:O    | 1:A:549:LYS:HE2   | 2.16        | 0.45     |
| 3:C:49:LEU:HG    | 4:D:55:LEU:HD12   | 1.98        | 0.45     |
| 1:A:536:ASP:O    | 1:A:539:CYS:HB2   | 2.16        | 0.45     |
| 4:D:24:SER:O     | 4:D:28:ALA:HB3    | 2.15        | 0.45     |
| 1:M:396:LEU:HG   | 11:M:821:FAD:C2   | 2.46        | 0.45     |
| 4:D:48:ALA:HA    | 4:D:53:ARG:HD3    | 1.98        | 0.45     |
| 2:N:39:ALA:O     | 2:N:43:ILE:HG12   | 2.16        | 0.45     |
| 1:A:202:ASN:HA   | 1:A:353:THR:HG22  | 1.99        | 0.45     |
| 1:A:176:MET:HG3  | 3:C:4:ARG:HD3     | 1.98        | 0.45     |
| 4:P:95:ALA:HB1   | 4:P:98:TRP:HB2    | 1.98        | 0.45     |
| 1:M:279:ASN:O    | 1:M:280:LYS:HB2   | 2.17        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:546:ASN:O    | 1:M:549:LYS:HE3  | 2.17        | 0.45     |
| 1:M:158:LEU:O    | 1:M:159:ASP:HB2  | 2.17        | 0.45     |
| 1:A:342:ASP:C    | 1:A:344:VAL:H    | 2.20        | 0.45     |
| 1:M:162:VAL:HG13 | 1:M:166:HIS:C    | 2.37        | 0.45     |
| 1:M:93:MET:HB3   | 1:M:125:TRP:CE3  | 2.50        | 0.45     |
| 3:O:36:VAL:HG23  | 3:O:37:TRP:N     | 2.32        | 0.45     |
| 4:P:9:ASP:N      | 4:P:9:ASP:OD2    | 2.49        | 0.45     |
| 1:A:366:ASN:O    | 1:A:367:CYS:HB2  | 2.16        | 0.45     |
| 1:A:317:ARG:O    | 1:A:319:LEU:N    | 2.50        | 0.45     |
| 1:A:385:LEU:HD23 | 1:A:386:HIS:CE1  | 2.52        | 0.45     |
| 1:M:498:PHE:CD2  | 2:N:103:VAL:HG21 | 2.51        | 0.45     |
| 1:M:320:GLY:O    | 1:M:324:LEU:HB2  | 2.17        | 0.45     |
| 1:A:332:CYS:O    | 1:A:336:LYS:HG3  | 2.17        | 0.45     |
| 1:M:114:ARG:C    | 1:M:122:GLU:HB2  | 2.36        | 0.45     |
| 3:C:90:ALA:N     | 3:C:91:PRO:CD    | 2.80        | 0.45     |
| 2:N:12:ARG:NH2   | 2:N:101:ASP:OD1  | 2.49        | 0.45     |
| 4:D:86:MET:CE    | 4:D:91:ILE:HD12  | 2.47        | 0.45     |
| 1:A:448:TRP:CG   | 1:A:449:ALA:N    | 2.85        | 0.45     |
| 1:A:141:GLN:HB3  | 2:B:118:PRO:O    | 2.17        | 0.45     |
| 4:P:51:TYR:CD1   | 4:P:52:GLU:N     | 2.82        | 0.44     |
| 1:M:488:ARG:HB3  | 1:M:488:ARG:CZ   | 2.46        | 0.44     |
| 4:P:30:VAL:O     | 4:P:33:LEU:HB3   | 2.17        | 0.44     |
| 2:N:235:PHE:CE1  | 4:P:9:ASP:HA     | 2.51        | 0.44     |
| 4:D:64:ARG:HH12  | 4:D:117:THR:HG23 | 1.82        | 0.44     |
| 2:N:162:GLY:HA3  | 3:O:11:MET:CE    | 2.47        | 0.44     |
| 1:A:45:THR:O     | 1:A:132:GLY:HA3  | 2.16        | 0.44     |
| 2:N:119:TYR:CE1  | 2:N:121:ILE:HD11 | 2.52        | 0.44     |
| 1:M:239:SER:OG   | 1:M:241:ILE:HG13 | 2.17        | 0.44     |
| 2:N:155:TYR:CZ   | 2:N:169:GLY:HA3  | 2.53        | 0.44     |
| 2:B:7:LYS:HE2    | 2:B:25:PHE:CD2   | 2.52        | 0.44     |
| 1:A:93:MET:HB3   | 1:A:125:TRP:CZ3  | 2.52        | 0.44     |
| 1:M:17:LEU:O     | 1:M:21:ILE:HG13  | 2.18        | 0.44     |
| 1:M:9:ILE:HD13   | 1:M:19:ALA:HB3   | 2.00        | 0.44     |
| 1:M:38:VAL:O     | 1:M:39:TYR:C     | 2.56        | 0.44     |
| 1:M:96:LEU:HD23  | 1:M:96:LEU:HA    | 1.86        | 0.44     |
| 1:A:0:MET:SD     | 1:A:182:GLN:HG3  | 2.58        | 0.44     |
| 1:M:102:PRO:HB2  | 2:N:139:MET:HE3  | 1.99        | 0.44     |
| 1:M:326:GLU:HG2  | 1:M:326:GLU:O    | 2.18        | 0.44     |
| 3:C:123:ILE:HD12 | 4:D:30:VAL:HG11  | 2.00        | 0.44     |
| 4:D:92:HIS:HB3   | 2:N:243:ARG:CB   | 2.48        | 0.44     |
| 3:O:114:ALA:O    | 3:O:118:VAL:HG23 | 2.18        | 0.44     |
| 1:M:41:MET:CE    | 2:N:150:ASN:HD22 | 2.31        | 0.44     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:P:64:ARG:O     | 4:P:115:VAL:HG21  | 2.17        | 0.44     |
| 1:A:324:LEU:HD23 | 1:A:328:LEU:HD12  | 2.00        | 0.44     |
| 1:A:356:TYR:HE1  | 11:A:721:FAD:O3'  | 2.01        | 0.43     |
| 1:M:44:HIS:NE2   | 11:M:821:FAD:HM81 | 2.18        | 0.43     |
| 1:M:488:ARG:CB   | 1:M:488:ARG:HH11  | 2.29        | 0.43     |
| 2:B:209:TYR:CZ   | 3:C:19:LEU:HD21   | 2.53        | 0.43     |
| 4:P:55:LEU:HD12  | 4:P:118:ILE:HD11  | 1.99        | 0.43     |
| 1:M:89:CYS:N     | 1:M:90:PRO:CD     | 2.78        | 0.43     |
| 1:M:171:VAL:CB   | 1:M:432:VAL:HG11  | 2.48        | 0.43     |
| 3:O:84:LYS:HE2   | 3:O:88:GLU:OE2    | 2.17        | 0.43     |
| 1:M:546:ASN:N    | 1:M:546:ASN:ND2   | 2.66        | 0.43     |
| 1:M:335:ALA:HA   | 1:M:339:VAL:HG22  | 2.00        | 0.43     |
| 1:M:435:ARG:O    | 1:M:435:ARG:HD2   | 2.18        | 0.43     |
| 1:M:46:VAL:HG23  | 1:M:133:PHE:HA    | 2.00        | 0.43     |
| 1:A:244:THR:HG22 | 1:A:331:ILE:CG1   | 2.49        | 0.43     |
| 4:D:114:GLY:O    | 4:D:117:THR:HA    | 2.18        | 0.43     |
| 1:M:548:LEU:HD12 | 1:M:568:VAL:HG21  | 1.99        | 0.43     |
| 1:M:382:SER:O    | 1:M:384:GLY:N     | 2.51        | 0.43     |
| 1:A:232:HIS:CD2  | 1:A:234:THR:H     | 2.33        | 0.43     |
| 1:M:21:ILE:O     | 1:M:25:GLN:HG3    | 2.19        | 0.43     |
| 1:M:329:PRO:HG2  | 1:M:330:PHE:H     | 1.83        | 0.43     |
| 2:N:155:TYR:CE2  | 2:N:169:GLY:HA3   | 2.54        | 0.43     |
| 2:B:136:PRO:HB2  | 3:C:100:ASP:OD1   | 2.17        | 0.43     |
| 3:C:37:TRP:CZ2   | 3:C:41:GLU:OE1    | 2.72        | 0.43     |
| 2:N:75:LEU:HD11  | 2:N:215:PRO:HG3   | 2.00        | 0.43     |
| 2:N:197:SER:HB2  | 4:P:5:PRO:HG2     | 2.00        | 0.43     |
| 1:A:328:LEU:N    | 1:A:329:PRO:CD    | 2.81        | 0.43     |
| 1:A:273:PRO:O    | 1:A:274:LEU:C     | 2.57        | 0.43     |
| 1:A:289:LYS:HZ3  | 14:A:705:1PE:H262 | 1.84        | 0.43     |
| 1:M:311:VAL:CG1  | 1:M:312:VAL:N     | 2.81        | 0.43     |
| 1:A:253:ILE:HG13 | 1:A:315:ASP:HB3   | 1.99        | 0.43     |
| 2:N:35:SER:O     | 2:N:38:ASP:HB2    | 2.19        | 0.43     |
| 2:N:149:ILE:HG23 | 2:N:216:LYS:HG3   | 1.99        | 0.43     |
| 2:N:221:ALA:O    | 2:N:225:GLN:HG2   | 2.19        | 0.43     |
| 1:M:239:SER:CB   | 1:M:241:ILE:HG13  | 2.49        | 0.43     |
| 2:N:82:ARG:HG3   | 2:N:83:ASP:OD1    | 2.19        | 0.43     |
| 1:A:204:ASN:HD22 | 1:A:204:ASN:N     | 2.17        | 0.43     |
| 3:C:49:LEU:HG    | 4:D:55:LEU:CD1    | 2.49        | 0.43     |
| 2:B:73:PRO:HG2   | 2:B:213:VAL:HG11  | 2.01        | 0.43     |
| 2:N:57:CYS:O     | 2:N:59:MET:HG2    | 2.19        | 0.43     |
| 4:D:53:ARG:HG2   | 4:D:53:ARG:HH11   | 1.84        | 0.43     |
| 1:M:382:SER:C    | 1:M:384:GLY:N     | 2.73        | 0.43     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:M:0:MET:O      | 1:M:1:GLN:HB2     | 2.19        | 0.42     |
| 2:N:135:THR:HG22 | 2:N:137:ALA:N     | 2.33        | 0.42     |
| 1:M:499:ASN:C    | 1:M:499:ASN:ND2   | 2.72        | 0.42     |
| 2:N:36:LEU:HD23  | 2:N:76:ALA:CB     | 2.49        | 0.42     |
| 1:A:78:GLU:OE2   | 1:A:568:VAL:HA    | 2.19        | 0.42     |
| 1:A:346:GLU:HB3  | 1:A:347:PRO:CD    | 2.49        | 0.42     |
| 2:N:81:LEU:CD1   | 2:N:81:LEU:N      | 2.82        | 0.42     |
| 4:D:4:ASN:HD21   | 4:P:6:LYS:HE3     | 1.84        | 0.42     |
| 2:N:110:ILE:O    | 2:N:114:GLU:HG3   | 2.19        | 0.42     |
| 1:A:89:CYS:N     | 1:A:90:PRO:CD     | 2.81        | 0.42     |
| 4:D:64:ARG:NH1   | 4:D:115:VAL:O     | 2.51        | 0.42     |
| 1:M:44:HIS:NE2   | 11:M:821:FAD:C8   | 2.78        | 0.42     |
| 2:B:188:LYS:NZ   | 2:B:230:GLU:CG    | 2.81        | 0.42     |
| 4:P:35:VAL:O     | 4:P:40:PRO:HD3    | 2.19        | 0.42     |
| 1:A:120:LYS:HG2  | 1:A:121:ILE:HD13  | 2.01        | 0.42     |
| 1:A:243:MET:HA   | 1:A:331:ILE:HD12  | 2.01        | 0.42     |
| 4:D:30:VAL:HG13  | 4:D:31:MET:N      | 2.34        | 0.42     |
| 1:M:548:LEU:HD21 | 1:M:575:PRO:HG3   | 2.02        | 0.42     |
| 4:P:68:PHE:CE1   | 4:P:72:VAL:HG21   | 2.55        | 0.42     |
| 4:P:10:GLU:OE2   | 4:P:80:HIS:HE1    | 2.02        | 0.42     |
| 1:M:365:GLN:O    | 1:M:366:ASN:ND2   | 2.48        | 0.42     |
| 1:M:481:GLU:O    | 1:M:485:ARG:HG2   | 2.18        | 0.42     |
| 4:D:36:GLY:C     | 4:D:37:ILE:HG13   | 2.40        | 0.42     |
| 1:A:379:GLU:HB2  | 11:A:721:FAD:H5'2 | 2.02        | 0.42     |
| 1:M:469:PRO:CD   | 1:M:536:ASP:HB3   | 2.50        | 0.42     |
| 1:M:469:PRO:HA   | 1:M:523:MET:HE3   | 2.02        | 0.42     |
| 1:A:42:ARG:HD2   | 1:A:42:ARG:N      | 2.35        | 0.42     |
| 2:N:137:ALA:HB2  | 3:O:100:ASP:OD1   | 2.20        | 0.42     |
| 2:B:6:LEU:HD23   | 2:B:81:LEU:HD13   | 2.02        | 0.42     |
| 3:O:59:PHE:O     | 3:O:62:PHE:HB3    | 2.20        | 0.42     |
| 2:N:54:ARG:HH21  | 2:N:103:VAL:CG1   | 2.33        | 0.42     |
| 1:M:92:GLU:HG3   | 1:M:400:VAL:O     | 2.20        | 0.42     |
| 1:M:100:GLY:O    | 2:N:184:ARG:NH2   | 2.51        | 0.42     |
| 1:M:85:PHE:CD2   | 1:M:385:LEU:HD11  | 2.55        | 0.42     |
| 2:N:45:ASP:OD1   | 7:N:803:ACT:H1    | 2.20        | 0.42     |
| 1:M:51:GLY:O     | 1:M:396:LEU:HD12  | 2.19        | 0.42     |
| 2:N:206:PHE:HA   | 9:N:245:F3S:S1    | 2.60        | 0.42     |
| 1:M:321:GLU:HA   | 1:M:324:LEU:HB3   | 2.02        | 0.42     |
| 1:A:542:ARG:NH2  | 1:A:544:ASP:OD2   | 2.41        | 0.42     |
| 1:M:184:ARG:HG3  | 1:M:184:ARG:HH11  | 1.85        | 0.42     |
| 1:M:370:ARG:HH12 | 1:M:554:PHE:HZ    | 1.67        | 0.42     |
| 1:M:18:ARG:HG2   | 1:M:400:VAL:HA    | 2.01        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:28:VAL:HA     | 2:B:29:PRO:HD3    | 1.92        | 0.41     |
| 2:N:72:VAL:HA     | 2:N:73:PRO:HD3    | 1.77        | 0.41     |
| 2:N:188:LYS:HE2   | 2:N:192:MET:CE    | 2.50        | 0.41     |
| 1:M:213:MET:HE3   | 1:M:380:CYS:HA    | 2.02        | 0.41     |
| 1:M:377:VAL:HG21  | 1:M:402:PHE:O     | 2.19        | 0.41     |
| 3:O:28:ARG:HD2    | 4:P:81:ARG:HH22   | 1.85        | 0.41     |
| 2:B:8:ILE:HD11    | 2:B:81:LEU:CD1    | 2.50        | 0.41     |
| 3:C:39:SER:O      | 3:C:43:ILE:HG13   | 2.21        | 0.41     |
| 1:A:68:ASP:HB3    | 1:A:391:LEU:HD21  | 2.01        | 0.41     |
| 2:N:16:GLU:HG2    | 3:O:3:LYS:HG2     | 2.02        | 0.41     |
| 1:A:242:LEU:HD21  | 6:A:702:OAA:O1    | 2.20        | 0.41     |
| 1:M:180:LEU:HD21  | 1:M:436:LEU:CD2   | 2.51        | 0.41     |
| 3:C:59:PHE:CZ     | 3:C:63:LEU:HD11   | 2.55        | 0.41     |
| 1:M:9:ILE:HD12    | 1:M:20:ALA:HB2    | 2.03        | 0.41     |
| 1:M:106:ARG:NH1   | 1:M:111:VAL:O     | 2.53        | 0.41     |
| 2:N:126:THR:OG1   | 2:N:129:GLN:HG3   | 2.21        | 0.41     |
| 3:C:50:LYS:HE2    | 3:C:50:LYS:CA     | 2.49        | 0.41     |
| 2:N:151:CYS:HB2   | 2:N:153:LEU:HG    | 2.03        | 0.41     |
| 4:P:96:GLY:O      | 4:P:97:LYS:C      | 2.57        | 0.41     |
| 1:M:48:ALA:HB3    | 1:M:132:GLY:HA3   | 2.02        | 0.41     |
| 3:C:12:THR:CG2    | 3:C:13:SER:N      | 2.83        | 0.41     |
| 4:P:72:VAL:HG12   | 4:P:76:TRP:CD1    | 2.56        | 0.41     |
| 3:C:15:TRP:CD2    | 3:C:16:TRP:N      | 2.88        | 0.41     |
| 1:M:527:GLU:OE2   | 1:M:529:ARG:NH1   | 2.54        | 0.41     |
| 1:A:443:ASP:HA    | 1:A:490:ARG:HG3   | 2.03        | 0.41     |
| 1:A:209:THR:OG1   | 1:A:507:GLU:HG2   | 2.20        | 0.41     |
| 1:M:439:LEU:O     | 1:M:442:GLN:HB3   | 2.20        | 0.41     |
| 1:M:342:ASP:HA    | 1:M:343:PRO:HD3   | 1.84        | 0.41     |
| 1:M:199:TYR:OH    | 1:M:229:VAL:HG21  | 2.21        | 0.41     |
| 2:N:150:ASN:HA    | 10:N:246:SF4:S4   | 2.61        | 0.41     |
| 13:P:710:CE1:H171 | 13:P:710:CE1:H211 | 2.02        | 0.41     |
| 1:M:570:ILE:HG22  | 1:M:571:THR:N     | 2.35        | 0.41     |
| 3:C:72:ASN:HA     | 3:C:72:ASN:HD22   | 1.61        | 0.41     |
| 1:M:316:LEU:O     | 1:M:319:LEU:HG    | 2.21        | 0.41     |
| 2:N:214:CYS:SG    | 2:N:218:VAL:HG23  | 2.60        | 0.41     |
| 2:B:188:LYS:HZ2   | 2:B:230:GLU:CG    | 2.34        | 0.41     |
| 3:O:89:LEU:C      | 3:O:91:PRO:HD2    | 2.41        | 0.41     |
| 1:M:26:ALA:O      | 1:M:28:PRO:HD3    | 2.21        | 0.41     |
| 1:M:233:PRO:HG2   | 1:M:248:ARG:NH2   | 2.36        | 0.41     |
| 1:M:233:PRO:HG2   | 1:M:248:ARG:HH22  | 1.84        | 0.41     |
| 3:O:47:PHE:HE2    | 4:P:114:GLY:HA3   | 1.86        | 0.41     |
| 1:A:59:HIS:H      | 1:A:59:HIS:CD2    | 2.39        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:7:LEU:CD2    | 1:M:411:THR:HA   | 2.39        | 0.41     |
| 2:B:134:GLN:HE21 | 2:B:139:MET:CE   | 2.35        | 0.41     |
| 1:M:62:PHE:HB3   | 1:M:86:VAL:CG2   | 2.50        | 0.41     |
| 1:A:204:ASN:ND2  | 1:A:204:ASN:N    | 2.69        | 0.41     |
| 1:A:57:GLN:NE2   | 1:A:122:GLU:HG2  | 2.36        | 0.41     |
| 1:M:485:ARG:HH11 | 1:M:485:ARG:HB3  | 1.85        | 0.40     |
| 2:N:56:SER:O     | 2:N:58:ARG:HG3   | 2.21        | 0.40     |
| 3:C:18:LYS:HB2   | 3:C:19:LEU:H     | 1.61        | 0.40     |
| 4:P:26:ILE:HG22  | 4:P:27:ILE:N     | 2.35        | 0.40     |
| 1:M:212:GLY:HA2  | 1:M:215:MET:HE2  | 2.03        | 0.40     |
| 1:M:356:TYR:HD1  | 1:M:358:MET:HG2  | 1.86        | 0.40     |
| 1:A:529:ARG:NH1  | 1:A:542:ARG:HG2  | 2.36        | 0.40     |
| 1:M:208:VAL:O    | 1:M:208:VAL:HG12 | 2.19        | 0.40     |
| 1:A:48:ALA:HA    | 11:A:721:FAD:C6  | 2.51        | 0.40     |
| 1:M:311:VAL:HG13 | 1:M:350:VAL:N    | 2.36        | 0.40     |
| 1:M:324:LEU:O    | 1:M:328:LEU:N    | 2.47        | 0.40     |
| 1:M:213:MET:HB3  | 1:M:223:LEU:HD21 | 2.04        | 0.40     |
| 2:B:141:LYS:HE3  | 3:C:95:ASN:OD1   | 2.21        | 0.40     |
| 4:D:95:ALA:HB2   | 2:N:239:THR:HG22 | 2.03        | 0.40     |
| 1:M:508:LEU:HD12 | 1:M:508:LEU:O    | 2.21        | 0.40     |
| 3:C:65:ASN:HB3   | 3:C:68:ILE:H     | 1.86        | 0.40     |
| 2:N:116:ILE:O    | 2:N:116:ILE:HG22 | 2.21        | 0.40     |
| 1:M:313:TYR:CD1  | 1:M:347:PRO:HB2  | 2.57        | 0.40     |
| 1:M:76:LEU:HD23  | 1:M:76:LEU:HA    | 1.98        | 0.40     |
| 1:A:152:PHE:HB3  | 1:A:155:HIS:CG   | 2.56        | 0.40     |
| 2:N:226:GLN:HB2  | 2:N:226:GLN:HE21 | 1.62        | 0.40     |
| 3:O:25:TYR:HD1   | 3:O:28:ARG:HH21  | 1.69        | 0.40     |
| 1:M:6:ASP:O      | 1:M:185:ALA:HB1  | 2.21        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 1   | A     | 575/602 (96%) | 541 (94%) | 30 (5%) | 4 (1%)   | 30 62       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | M     | 575/602 (96%)   | 487 (85%)  | 75 (13%) | 13 (2%)  | 10          | 24 |
| 2   | B     | 241/243 (99%)   | 224 (93%)  | 16 (7%)  | 1 (0%)   | 43          | 76 |
| 2   | N     | 241/243 (99%)   | 215 (89%)  | 20 (8%)  | 6 (2%)   | 9           | 21 |
| 3   | C     | 128/130 (98%)   | 120 (94%)  | 4 (3%)   | 4 (3%)   | 7           | 14 |
| 3   | O     | 128/130 (98%)   | 114 (89%)  | 12 (9%)  | 2 (2%)   | 14          | 35 |
| 4   | D     | 117/119 (98%)   | 111 (95%)  | 3 (3%)   | 3 (3%)   | 8           | 20 |
| 4   | P     | 117/119 (98%)   | 102 (87%)  | 14 (12%) | 1 (1%)   | 25          | 55 |
| All | All   | 2122/2188 (97%) | 1914 (90%) | 174 (8%) | 34 (2%)  | 14          | 35 |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 18  | LYS  |
| 3   | C     | 65  | ASN  |
| 1   | M     | 244 | THR  |
| 1   | M     | 382 | SER  |
| 1   | A     | 318 | HIS  |
| 1   | M     | 79  | GLN  |
| 1   | M     | 540 | THR  |
| 2   | N     | 183 | SER  |
| 3   | O     | 18  | LYS  |
| 2   | B     | 56  | SER  |
| 4   | D     | 43  | LEU  |
| 1   | A     | 389 | ASN  |
| 3   | C     | 66  | PRO  |
| 1   | M     | 329 | PRO  |
| 1   | M     | 492 | THR  |
| 2   | N     | 55  | TRP  |
| 2   | N     | 93  | LEU  |
| 2   | N     | 101 | ASP  |
| 3   | O     | 99  | LYS  |
| 1   | A     | 244 | THR  |
| 1   | M     | 119 | MET  |
| 1   | M     | 257 | LYS  |
| 1   | M     | 344 | VAL  |
| 2   | N     | 56  | SER  |
| 1   | A     | 343 | PRO  |
| 4   | D     | 117 | THR  |
| 1   | M     | 318 | HIS  |
| 1   | M     | 324 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 128 | ASP  |
| 1   | M     | 444 | GLY  |
| 4   | P     | 4   | ASN  |
| 1   | M     | 383 | VAL  |
| 3   | C     | 104 | GLY  |
| 4   | D     | 99  | 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     | 460/475 (97%)   | 446 (97%)  | 14 (3%)  | 53          | 84 |
| 1   | M     | 460/475 (97%)   | 437 (95%)  | 23 (5%)  | 34          | 66 |
| 2   | B     | 205/205 (100%)  | 199 (97%)  | 6 (3%)   | 55          | 85 |
| 2   | N     | 205/205 (100%)  | 195 (95%)  | 10 (5%)  | 35          | 67 |
| 3   | C     | 111/111 (100%)  | 107 (96%)  | 4 (4%)   | 47          | 79 |
| 3   | O     | 111/111 (100%)  | 108 (97%)  | 3 (3%)   | 57          | 87 |
| 4   | D     | 97/97 (100%)    | 94 (97%)   | 3 (3%)   | 52          | 83 |
| 4   | P     | 97/97 (100%)    | 95 (98%)   | 2 (2%)   | 66          | 91 |
| All | All   | 1746/1776 (98%) | 1681 (96%) | 65 (4%)  | 45          | 78 |

All (65) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 42  | ARG  |
| 1   | A     | 74  | ASP  |
| 1   | A     | 93  | MET  |
| 1   | A     | 184 | ARG  |
| 1   | A     | 197 | ARG  |
| 1   | A     | 200 | ARG  |
| 1   | A     | 319 | LEU  |
| 1   | A     | 325 | HIS  |
| 1   | A     | 327 | ARG  |
| 1   | A     | 358 | MET  |
| 1   | A     | 413 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 498 | PHE  |
| 1   | A     | 528 | SER  |
| 1   | A     | 560 | THR  |
| 2   | B     | 65  | CYS  |
| 2   | B     | 81  | LEU  |
| 2   | B     | 128 | ASP  |
| 2   | B     | 178 | ARG  |
| 2   | B     | 206 | PHE  |
| 2   | B     | 212 | GLU  |
| 3   | C     | 39  | SER  |
| 3   | C     | 50  | LYS  |
| 3   | C     | 84  | LYS  |
| 3   | C     | 92  | LYS  |
| 4   | D     | 0   | MET  |
| 4   | D     | 86  | MET  |
| 4   | D     | 118 | ILE  |
| 1   | M     | 74  | ASP  |
| 1   | M     | 93  | MET  |
| 1   | M     | 122 | GLU  |
| 1   | M     | 126 | PHE  |
| 1   | M     | 137 | HIS  |
| 1   | M     | 143 | SER  |
| 1   | M     | 155 | HIS  |
| 1   | M     | 156 | PHE  |
| 1   | M     | 163 | ASP  |
| 1   | M     | 164 | ASP  |
| 1   | M     | 197 | ARG  |
| 1   | M     | 227 | GLU  |
| 1   | M     | 243 | MET  |
| 1   | M     | 330 | PHE  |
| 1   | M     | 375 | PHE  |
| 1   | M     | 389 | ASN  |
| 1   | M     | 413 | ARG  |
| 1   | M     | 465 | ILE  |
| 1   | M     | 470 | GLU  |
| 1   | M     | 485 | ARG  |
| 1   | M     | 498 | PHE  |
| 1   | M     | 499 | ASN  |
| 1   | M     | 558 | ASP  |
| 2   | N     | 46  | ASN  |
| 2   | N     | 50  | ASP  |
| 2   | N     | 100 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 128 | ASP  |
| 2   | N     | 148 | CYS  |
| 2   | N     | 178 | ARG  |
| 2   | N     | 185 | ASP  |
| 2   | N     | 189 | LYS  |
| 2   | N     | 206 | PHE  |
| 2   | N     | 226 | GLN  |
| 3   | O     | 5   | LYS  |
| 3   | O     | 37  | TRP  |
| 3   | O     | 39  | SER  |
| 4   | P     | 7   | ARG  |
| 4   | P     | 51  | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | HIS  |
| 1   | A     | 141 | GLN  |
| 1   | A     | 232 | HIS  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 292 | GLN  |
| 1   | A     | 434 | GLN  |
| 1   | A     | 442 | GLN  |
| 2   | B     | 134 | GLN  |
| 2   | B     | 194 | GLN  |
| 3   | C     | 51  | ASN  |
| 3   | C     | 72  | ASN  |
| 4   | D     | 4   | ASN  |
| 4   | D     | 59  | GLN  |
| 1   | M     | 1   | GLN  |
| 1   | M     | 27  | ASN  |
| 1   | M     | 137 | HIS  |
| 1   | M     | 174 | ASN  |
| 1   | M     | 204 | ASN  |
| 1   | M     | 292 | GLN  |
| 1   | M     | 394 | ASN  |
| 1   | M     | 409 | GLN  |
| 1   | M     | 421 | ASN  |
| 1   | M     | 434 | GLN  |
| 1   | M     | 441 | ASN  |
| 1   | M     | 447 | ASN  |
| 1   | M     | 499 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 520 | HIS  |
| 1   | M     | 546 | ASN  |
| 2   | N     | 95  | ASN  |
| 2   | N     | 129 | GLN  |
| 2   | N     | 150 | ASN  |
| 2   | N     | 160 | GLN  |
| 2   | N     | 177 | HIS  |
| 2   | N     | 186 | HIS  |
| 2   | N     | 226 | GLN  |
| 3   | O     | 72  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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 | $\# Z  > 2$ |
| 6   | OAA  | A     | 702 | -    | 6,8,8        | 1.34 | 1 (16%)     | 7,10,10     | 1.71 | 2 (28%)     |
| 7   | ACT  | A     | 703 | -    | 1,3,3        | 1.68 | 0           | 0,3,3       | 0.00 | -           |
| 14  | 1PE  | A     | 705 | -    | 15,15,15     | 1.62 | 0           | 14,14,14    | 2.18 | 8 (57%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |       |           | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|-------|-----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ  | # Z  > 2  | Counts      | RMSZ | # Z  > 2 |
| 11  | FAD  | A     | 721 | -    | 58,58,58     | 1.67  | 10 (17%)  | 85,89,89    | 2.04 | 14 (16%) |
| 8   | FES  | B     | 244 | 2    | 0,4,4        | 0.00  | -         | 0,4,4       | 0.00 | -        |
| 9   | F3S  | B     | 245 | 2    | 3,9,9        | 14.65 | 3 (100%)  | 0,15,15     | 0.00 | -        |
| 10  | SF4  | B     | 246 | 2    | 12,12,12     | 28.16 | 12 (100%) | 0,24,24     | 0.00 | -        |
| 7   | ACT  | B     | 704 | -    | 1,3,3        | 2.86  | 1 (100%)  | 0,3,3       | 0.00 | -        |
| 12  | HQO  | C     | 700 | -    | 20,20,20     | 1.87  | 7 (35%)   | 26,26,26    | 1.02 | 1 (3%)   |
| 6   | OAA  | M     | 802 | -    | 6,8,8        | 1.31  | 1 (16%)   | 7,10,10     | 1.72 | 2 (28%)  |
| 11  | FAD  | M     | 821 | -    | 58,58,58     | 1.49  | 12 (20%)  | 85,89,89    | 2.08 | 11 (12%) |
| 8   | FES  | N     | 244 | 2    | 0,4,4        | 0.00  | -         | 0,4,4       | 0.00 | -        |
| 9   | F3S  | N     | 245 | 2    | 3,9,9        | 11.71 | 2 (66%)   | 0,15,15     | 0.00 | -        |
| 10  | SF4  | N     | 246 | 2    | 12,12,12     | 62.27 | 12 (100%) | 0,24,24     | 0.00 | -        |
| 12  | HQO  | N     | 800 | -    | 20,20,20     | 1.87  | 7 (35%)   | 26,26,26    | 1.02 | 1 (3%)   |
| 7   | ACT  | N     | 803 | -    | 1,3,3        | 2.65  | 1 (100%)  | 0,3,3       | 0.00 | -        |
| 13  | CE1  | O     | 811 | -    | 36,36,36     | 1.10  | 0         | 35,35,35    | 1.95 | 16 (45%) |
| 13  | CE1  | O     | 812 | -    | 36,36,36     | 1.10  | 0         | 35,35,35    | 1.87 | 16 (45%) |
| 13  | CE1  | O     | 813 | -    | 36,36,36     | 1.17  | 0         | 35,35,35    | 1.93 | 16 (45%) |
| 13  | CE1  | P     | 710 | -    | 36,36,36     | 1.09  | 0         | 35,35,35    | 1.89 | 16 (45%) |
| 13  | CE1  | P     | 810 | -    | 36,36,36     | 1.09  | 0         | 35,35,35    | 1.97 | 16 (45%) |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 6   | OAA  | A     | 702 | -    | -       | 0/6/8/8    | 0/0/0/0 |
| 7   | ACT  | A     | 703 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 14  | 1PE  | A     | 705 | -    | -       | 0/13/13/13 | 0/0/0/0 |
| 11  | FAD  | A     | 721 | -    | -       | 0/34/50/50 | 0/1/6/6 |
| 8   | FES  | B     | 244 | 2    | -       | 0/0/4/4    | 0/0/1/1 |
| 9   | F3S  | B     | 245 | 2    | -       | 0/0/24/24  | 0/0/3/3 |
| 10  | SF4  | B     | 246 | 2    | -       | 0/0/48/48  | 0/0/5/5 |
| 7   | ACT  | B     | 704 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 12  | HQO  | C     | 700 | -    | -       | 0/7/7/7    | 0/0/2/2 |
| 6   | OAA  | M     | 802 | -    | -       | 0/6/8/8    | 0/0/0/0 |
| 11  | FAD  | M     | 821 | -    | -       | 0/34/50/50 | 0/1/6/6 |
| 8   | FES  | N     | 244 | 2    | -       | 0/0/4/4    | 0/0/1/1 |
| 9   | F3S  | N     | 245 | 2    | -       | 0/0/24/24  | 0/0/3/3 |
| 10  | SF4  | N     | 246 | 2    | -       | 0/0/48/48  | 0/0/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 12  | HQO  | N     | 800 | -    | -       | 0/7/7/7    | 0/0/2/2 |
| 7   | ACT  | N     | 803 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 13  | CE1  | O     | 811 | -    | -       | 0/34/34/34 | 0/0/0/0 |
| 13  | CE1  | O     | 812 | -    | -       | 0/34/34/34 | 0/0/0/0 |
| 13  | CE1  | O     | 813 | -    | -       | 0/34/34/34 | 0/0/0/0 |
| 13  | CE1  | P     | 710 | -    | -       | 0/34/34/34 | 0/0/0/0 |
| 13  | CE1  | P     | 810 | -    | -       | 0/34/34/34 | 0/0/0/0 |

All (69) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 10  | N     | 246 | SF4  | S1-FE2  | 96.29  | 2.98        | 2.33     |
| 10  | N     | 246 | SF4  | S2-FE3  | -94.96 | 1.69        | 2.33     |
| 10  | N     | 246 | SF4  | S2-FE1  | 93.86  | 2.96        | 2.33     |
| 10  | N     | 246 | SF4  | S1-FE4  | -82.38 | 1.77        | 2.33     |
| 10  | N     | 246 | SF4  | S1-FE3  | -58.80 | 1.93        | 2.33     |
| 10  | N     | 246 | SF4  | S4-FE1  | -54.09 | 1.96        | 2.33     |
| 10  | B     | 246 | SF4  | S2-FE3  | -49.06 | 2.00        | 2.33     |
| 10  | B     | 246 | SF4  | S1-FE4  | -47.52 | 2.01        | 2.33     |
| 10  | N     | 246 | SF4  | S3-FE2  | -43.81 | 2.03        | 2.33     |
| 10  | B     | 246 | SF4  | S4-FE1  | -38.35 | 2.07        | 2.33     |
| 10  | N     | 246 | SF4  | S4-FE3  | 36.24  | 2.57        | 2.33     |
| 10  | N     | 246 | SF4  | S4-FE2  | -33.72 | 2.10        | 2.33     |
| 10  | N     | 246 | SF4  | S3-FE1  | -32.51 | 2.11        | 2.33     |
| 10  | B     | 246 | SF4  | S1-FE3  | -30.52 | 2.12        | 2.33     |
| 10  | B     | 246 | SF4  | S3-FE2  | -30.34 | 2.12        | 2.33     |
| 10  | B     | 246 | SF4  | S4-FE2  | -24.41 | 2.16        | 2.33     |
| 10  | N     | 246 | SF4  | S3-FE4  | 24.35  | 2.49        | 2.33     |
| 10  | B     | 246 | SF4  | S3-FE1  | -21.61 | 2.18        | 2.33     |
| 9   | B     | 245 | F3S  | S3-FE1  | -20.81 | 2.19        | 2.33     |
| 9   | N     | 245 | F3S  | S3-FE1  | -19.63 | 2.20        | 2.33     |
| 10  | N     | 246 | SF4  | S2-FE4  | -15.61 | 2.22        | 2.33     |
| 10  | B     | 246 | SF4  | S2-FE4  | -12.59 | 2.24        | 2.33     |
| 9   | B     | 245 | F3S  | S3-FE3  | -11.95 | 2.25        | 2.33     |
| 10  | B     | 246 | SF4  | S4-FE3  | -11.35 | 2.25        | 2.33     |
| 10  | B     | 246 | SF4  | S2-FE1  | -11.27 | 2.25        | 2.33     |
| 9   | B     | 245 | F3S  | S3-FE4  | -8.23  | 2.27        | 2.33     |
| 10  | B     | 246 | SF4  | S1-FE2  | -5.18  | 2.29        | 2.33     |
| 9   | N     | 245 | F3S  | S3-FE4  | -5.03  | 2.29        | 2.33     |
| 10  | B     | 246 | SF4  | S3-FE4  | 4.83   | 2.36        | 2.33     |
| 11  | A     | 721 | FAD  | C4A-N9A | -4.29  | 1.31        | 1.37     |
| 12  | N     | 800 | HQO  | C11-C3  | -3.98  | 1.42        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | C     | 700 | HQO  | C11-C3  | -3.97 | 1.42        | 1.50     |
| 11  | M     | 821 | FAD  | C9A-N10 | 3.83  | 1.44        | 1.38     |
| 11  | A     | 721 | FAD  | C4-N3   | 3.79  | 1.43        | 1.37     |
| 11  | A     | 721 | FAD  | C1'-C2' | 3.75  | 1.55        | 1.51     |
| 12  | C     | 700 | HQO  | O1-C1   | -3.46 | 1.26        | 1.35     |
| 12  | N     | 800 | HQO  | O1-C1   | -3.45 | 1.26        | 1.35     |
| 11  | A     | 721 | FAD  | C8A-N9A | -3.45 | 1.31        | 1.36     |
| 11  | M     | 821 | FAD  | C4A-N3A | 3.43  | 1.40        | 1.35     |
| 11  | M     | 821 | FAD  | O4B-C1B | 3.37  | 1.46        | 1.41     |
| 11  | A     | 721 | FAD  | P-O3P   | -3.32 | 1.53        | 1.59     |
| 11  | M     | 821 | FAD  | C5'-C4' | 3.17  | 1.56        | 1.51     |
| 11  | M     | 821 | FAD  | C4-N3   | 3.14  | 1.42        | 1.37     |
| 11  | A     | 721 | FAD  | PA-O3P  | -3.09 | 1.54        | 1.59     |
| 12  | N     | 800 | HQO  | O4-N1   | -3.08 | 1.23        | 1.30     |
| 12  | C     | 700 | HQO  | O4-N1   | -3.08 | 1.23        | 1.30     |
| 11  | A     | 721 | FAD  | C10-N10 | 2.89  | 1.45        | 1.38     |
| 11  | M     | 821 | FAD  | P-O3P   | -2.86 | 1.54        | 1.59     |
| 7   | B     | 704 | ACT  | CH3-C   | 2.86  | 1.52        | 1.48     |
| 7   | N     | 803 | ACT  | CH3-C   | 2.65  | 1.52        | 1.48     |
| 11  | M     | 821 | FAD  | C5X-N5  | 2.64  | 1.39        | 1.35     |
| 12  | N     | 800 | HQO  | C7-C6   | 2.53  | 1.42        | 1.36     |
| 12  | C     | 700 | HQO  | C7-C6   | 2.52  | 1.42        | 1.36     |
| 12  | N     | 800 | HQO  | C8-C9   | 2.42  | 1.42        | 1.36     |
| 11  | M     | 821 | FAD  | C1'-C2' | 2.42  | 1.53        | 1.51     |
| 12  | C     | 700 | HQO  | C8-C9   | 2.38  | 1.42        | 1.36     |
| 11  | M     | 821 | FAD  | PA-O3P  | -2.33 | 1.55        | 1.59     |
| 11  | A     | 721 | FAD  | C2B-C1B | -2.27 | 1.50        | 1.53     |
| 6   | A     | 702 | OAA  | C2-C1   | 2.19  | 1.51        | 1.49     |
| 12  | N     | 800 | HQO  | C2-C3   | 2.19  | 1.43        | 1.38     |
| 12  | C     | 700 | HQO  | C2-C3   | 2.17  | 1.43        | 1.38     |
| 11  | M     | 821 | FAD  | C1'-N10 | 2.17  | 1.50        | 1.48     |
| 6   | M     | 802 | OAA  | C2-C1   | 2.14  | 1.51        | 1.49     |
| 11  | A     | 721 | FAD  | C5A-N7A | -2.13 | 1.32        | 1.40     |
| 11  | M     | 821 | FAD  | C4A-N9A | -2.12 | 1.34        | 1.37     |
| 11  | M     | 821 | FAD  | C10-N10 | 2.10  | 1.43        | 1.38     |
| 11  | A     | 721 | FAD  | C6-C5X  | -2.04 | 1.39        | 1.41     |
| 12  | N     | 800 | HQO  | C8-C7   | 2.04  | 1.43        | 1.37     |
| 12  | C     | 700 | HQO  | C8-C7   | 2.03  | 1.43        | 1.37     |

All (119) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 11  | M     | 821 | FAD  | N3A-C2A-N1A | -10.73 | 119.73      | 128.71   |
| 11  | A     | 721 | FAD  | C2-N1-C10   | 8.02   | 123.06      | 114.98   |
| 11  | M     | 821 | FAD  | C2-N1-C10   | 6.84   | 121.87      | 114.98   |
| 11  | A     | 721 | FAD  | N3A-C2A-N1A | -6.62  | 123.17      | 128.71   |
| 11  | A     | 721 | FAD  | C4X-N5-C5X  | 5.70   | 123.09      | 116.69   |
| 11  | M     | 821 | FAD  | C4X-N5-C5X  | 5.63   | 123.02      | 116.69   |
| 11  | A     | 721 | FAD  | C4X-C10-N10 | -5.61  | 117.71      | 120.51   |
| 11  | M     | 821 | FAD  | C4X-C10-N10 | -5.12  | 117.95      | 120.51   |
| 11  | A     | 721 | FAD  | N3A-C4A-N9A | 4.82   | 134.14      | 125.43   |
| 11  | M     | 821 | FAD  | O4B-C1B-N9A | 4.82   | 112.92      | 108.44   |
| 11  | A     | 721 | FAD  | O4B-C1B-N9A | 4.70   | 112.82      | 108.44   |
| 11  | M     | 821 | FAD  | N3A-C4A-N9A | 4.60   | 133.73      | 125.43   |
| 13  | P     | 810 | CE1  | O28-C27-C26 | 4.59   | 131.30      | 110.47   |
| 11  | A     | 721 | FAD  | C4X-C10-N1  | -3.84  | 118.89      | 122.73   |
| 11  | M     | 821 | FAD  | C4-N3-C2    | -3.40  | 118.42      | 125.39   |
| 11  | A     | 721 | FAD  | C5'-C4'-C3' | 3.33   | 118.34      | 112.06   |
| 6   | M     | 802 | OAA  | C2-C3-C4    | -3.28  | 112.55      | 117.75   |
| 11  | A     | 721 | FAD  | P-O3P-PA    | 3.28   | 141.29      | 131.68   |
| 6   | A     | 702 | OAA  | C2-C3-C4    | -3.27  | 112.56      | 117.75   |
| 13  | O     | 813 | CE1  | O22-C23-C24 | 3.19   | 124.96      | 110.47   |
| 13  | O     | 811 | CE1  | O19-C18-C17 | 3.19   | 124.92      | 110.47   |
| 13  | O     | 813 | CE1  | O22-C21-C20 | 3.15   | 124.76      | 110.47   |
| 13  | P     | 710 | CE1  | O28-C27-C26 | 3.15   | 124.76      | 110.47   |
| 13  | O     | 812 | CE1  | O22-C21-C20 | 3.14   | 124.73      | 110.47   |
| 13  | O     | 812 | CE1  | O22-C23-C24 | 3.12   | 124.61      | 110.47   |
| 13  | O     | 812 | CE1  | O13-C14-C15 | 3.11   | 124.59      | 110.47   |
| 13  | P     | 810 | CE1  | O28-C29-C30 | 3.09   | 124.49      | 110.47   |
| 13  | P     | 810 | CE1  | O13-C14-C15 | 3.09   | 124.48      | 110.47   |
| 13  | P     | 710 | CE1  | O25-C24-C23 | 3.07   | 124.41      | 110.47   |
| 13  | O     | 811 | CE1  | O16-C17-C18 | 3.06   | 124.38      | 110.47   |
| 13  | O     | 811 | CE1  | O22-C23-C24 | 3.06   | 124.37      | 110.47   |
| 11  | A     | 721 | FAD  | C4-N3-C2    | -3.05  | 119.13      | 125.39   |
| 13  | O     | 811 | CE1  | O16-C15-C14 | 3.02   | 124.19      | 110.47   |
| 13  | O     | 812 | CE1  | O16-C15-C14 | 3.00   | 124.07      | 110.47   |
| 13  | P     | 710 | CE1  | O13-C14-C15 | 2.98   | 123.97      | 110.47   |
| 11  | M     | 821 | FAD  | P-O3P-PA    | 2.98   | 140.41      | 131.68   |
| 13  | P     | 810 | CE1  | O22-C23-C24 | 2.97   | 123.96      | 110.47   |
| 13  | O     | 813 | CE1  | O19-C18-C17 | 2.96   | 123.92      | 110.47   |
| 13  | P     | 710 | CE1  | O22-C23-C24 | 2.95   | 123.85      | 110.47   |
| 12  | C     | 700 | HQO  | O1-C1-C10   | 2.93   | 120.83      | 116.25   |
| 12  | N     | 800 | HQO  | O1-C1-C10   | 2.92   | 120.82      | 116.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | A     | 705 | 1PE  | OH5-C25-C15 | 2.91  | 123.65      | 110.47   |
| 13  | P     | 710 | CE1  | O34-C33-C32 | 2.89  | 123.60      | 110.47   |
| 13  | O     | 813 | CE1  | O25-C24-C23 | 2.87  | 123.49      | 110.47   |
| 13  | P     | 810 | CE1  | O25-C24-C23 | 2.86  | 123.46      | 110.47   |
| 13  | O     | 813 | CE1  | O16-C15-C14 | 2.86  | 123.43      | 110.47   |
| 13  | O     | 812 | CE1  | O19-C18-C17 | 2.85  | 123.40      | 110.47   |
| 13  | O     | 813 | CE1  | O25-C26-C27 | 2.83  | 123.31      | 110.47   |
| 11  | A     | 721 | FAD  | O3'-C3'-C2' | -2.83 | 101.58      | 108.74   |
| 13  | O     | 813 | CE1  | O31-C32-C33 | 2.82  | 123.25      | 110.47   |
| 11  | A     | 721 | FAD  | N1-C10-N10  | 2.81  | 123.37      | 115.97   |
| 13  | O     | 812 | CE1  | O34-C33-C32 | 2.79  | 123.15      | 110.47   |
| 13  | O     | 811 | CE1  | O31-C32-C33 | 2.79  | 123.11      | 110.47   |
| 14  | A     | 705 | 1PE  | OH4-C24-C14 | 2.77  | 123.03      | 110.47   |
| 13  | O     | 813 | CE1  | O28-C29-C30 | 2.76  | 123.01      | 110.47   |
| 13  | O     | 811 | CE1  | O19-C20-C21 | 2.76  | 122.99      | 110.47   |
| 14  | A     | 705 | 1PE  | OH4-C13-C23 | 2.75  | 122.95      | 110.47   |
| 13  | P     | 710 | CE1  | O16-C15-C14 | 2.73  | 122.84      | 110.47   |
| 13  | O     | 811 | CE1  | O22-C21-C20 | 2.71  | 122.77      | 110.47   |
| 13  | O     | 811 | CE1  | O25-C24-C23 | 2.71  | 122.75      | 110.47   |
| 13  | P     | 710 | CE1  | O19-C20-C21 | 2.69  | 122.68      | 110.47   |
| 13  | O     | 811 | CE1  | O34-C33-C32 | 2.69  | 122.68      | 110.47   |
| 13  | O     | 813 | CE1  | O34-C35-C36 | 2.69  | 123.52      | 110.61   |
| 13  | O     | 812 | CE1  | O16-C17-C18 | 2.67  | 122.57      | 110.47   |
| 13  | P     | 810 | CE1  | O34-C33-C32 | 2.67  | 122.57      | 110.47   |
| 13  | O     | 812 | CE1  | O31-C32-C33 | 2.67  | 122.57      | 110.47   |
| 13  | P     | 810 | CE1  | O31-C30-C29 | 2.65  | 122.50      | 110.47   |
| 13  | O     | 813 | CE1  | O13-C14-C15 | 2.63  | 122.41      | 110.47   |
| 13  | P     | 810 | CE1  | O22-C21-C20 | 2.61  | 122.32      | 110.47   |
| 13  | P     | 810 | CE1  | O16-C17-C18 | 2.60  | 122.28      | 110.47   |
| 13  | O     | 813 | CE1  | O34-C33-C32 | 2.60  | 122.25      | 110.47   |
| 13  | O     | 812 | CE1  | O31-C30-C29 | 2.57  | 122.14      | 110.47   |
| 14  | A     | 705 | 1PE  | OH3-C23-C13 | 2.57  | 122.14      | 110.47   |
| 13  | O     | 812 | CE1  | O25-C24-C23 | 2.57  | 122.11      | 110.47   |
| 13  | O     | 811 | CE1  | O28-C27-C26 | 2.56  | 122.10      | 110.47   |
| 14  | A     | 705 | 1PE  | OH6-C15-C25 | 2.55  | 122.04      | 110.47   |
| 13  | P     | 810 | CE1  | O19-C20-C21 | 2.55  | 122.03      | 110.47   |
| 13  | O     | 812 | CE1  | O34-C35-C36 | 2.55  | 122.85      | 110.61   |
| 13  | O     | 811 | CE1  | O13-C14-C15 | 2.54  | 121.98      | 110.47   |
| 13  | O     | 811 | CE1  | O31-C30-C29 | 2.53  | 121.95      | 110.47   |
| 14  | A     | 705 | 1PE  | OH3-C22-C12 | 2.53  | 122.76      | 110.61   |
| 13  | O     | 811 | CE1  | O28-C29-C30 | 2.52  | 121.88      | 110.47   |
| 13  | O     | 813 | CE1  | O28-C27-C26 | 2.50  | 121.82      | 110.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | P     | 710 | CE1  | O31-C30-C29 | 2.50  | 121.80      | 110.47   |
| 13  | O     | 813 | CE1  | O31-C30-C29 | 2.49  | 121.77      | 110.47   |
| 13  | O     | 813 | CE1  | O13-C12-C11 | 2.48  | 119.72      | 109.88   |
| 13  | P     | 710 | CE1  | O22-C21-C20 | 2.47  | 121.67      | 110.47   |
| 13  | P     | 710 | CE1  | O28-C29-C30 | 2.46  | 121.62      | 110.47   |
| 13  | P     | 810 | CE1  | O16-C15-C14 | 2.46  | 121.62      | 110.47   |
| 13  | O     | 811 | CE1  | O13-C12-C11 | 2.45  | 119.60      | 109.88   |
| 13  | P     | 710 | CE1  | O31-C32-C33 | 2.44  | 121.54      | 110.47   |
| 13  | O     | 811 | CE1  | O25-C26-C27 | 2.43  | 121.48      | 110.47   |
| 13  | P     | 710 | CE1  | O19-C18-C17 | 2.41  | 121.39      | 110.47   |
| 13  | O     | 811 | CE1  | O34-C35-C36 | 2.39  | 122.12      | 110.61   |
| 13  | P     | 710 | CE1  | O34-C35-C36 | 2.38  | 122.03      | 110.61   |
| 13  | P     | 710 | CE1  | O25-C26-C27 | 2.37  | 121.24      | 110.47   |
| 13  | P     | 810 | CE1  | O31-C32-C33 | 2.37  | 121.24      | 110.47   |
| 14  | A     | 705 | 1PE  | OH5-C14-C24 | 2.34  | 121.09      | 110.47   |
| 13  | P     | 710 | CE1  | O13-C12-C11 | 2.34  | 119.15      | 109.88   |
| 11  | A     | 721 | FAD  | C8A-N9A-C4A | 2.31  | 108.66      | 106.90   |
| 13  | O     | 812 | CE1  | O28-C27-C26 | 2.29  | 120.86      | 110.47   |
| 13  | P     | 810 | CE1  | O34-C35-C36 | 2.29  | 121.61      | 110.61   |
| 13  | O     | 812 | CE1  | O28-C29-C30 | 2.28  | 120.80      | 110.47   |
| 13  | O     | 813 | CE1  | O16-C17-C18 | 2.27  | 120.79      | 110.47   |
| 6   | M     | 802 | OAA  | O3-C3-C2    | 2.27  | 125.88      | 120.84   |
| 6   | A     | 702 | OAA  | O3-C3-C2    | 2.26  | 125.86      | 120.84   |
| 11  | M     | 821 | FAD  | C5'-C4'-C3' | 2.25  | 116.30      | 112.06   |
| 13  | O     | 812 | CE1  | O25-C26-C27 | 2.24  | 120.64      | 110.47   |
| 13  | P     | 710 | CE1  | O16-C17-C18 | 2.23  | 120.59      | 110.47   |
| 13  | O     | 812 | CE1  | O13-C12-C11 | 2.23  | 118.71      | 109.88   |
| 13  | O     | 812 | CE1  | O19-C20-C21 | 2.23  | 120.57      | 110.47   |
| 14  | A     | 705 | 1PE  | OH6-C26-C16 | 2.22  | 121.29      | 110.61   |
| 13  | P     | 810 | CE1  | O19-C18-C17 | 2.22  | 120.53      | 110.47   |
| 13  | P     | 810 | CE1  | O25-C26-C27 | 2.18  | 120.38      | 110.47   |
| 11  | M     | 821 | FAD  | O3P-P-O5'   | 2.18  | 113.15      | 103.41   |
| 13  | O     | 813 | CE1  | C10-C11-C12 | -2.16 | 103.11      | 113.58   |
| 11  | A     | 721 | FAD  | C5A-C4A-N3A | -2.13 | 121.06      | 125.70   |
| 13  | P     | 810 | CE1  | O13-C12-C11 | 2.06  | 118.06      | 109.88   |
| 11  | M     | 821 | FAD  | C2A-N3A-C4A | 2.04  | 119.81      | 114.01   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.