



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2021 – 12:16 PM EST

PDB ID : 5SUQ  
Title : Crystal structure of the THO-Sub2 complex  
Authors : Ren, Y.; Blobel, G.  
Deposited on : 2016-08-03  
Resolution : 6.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.17  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17

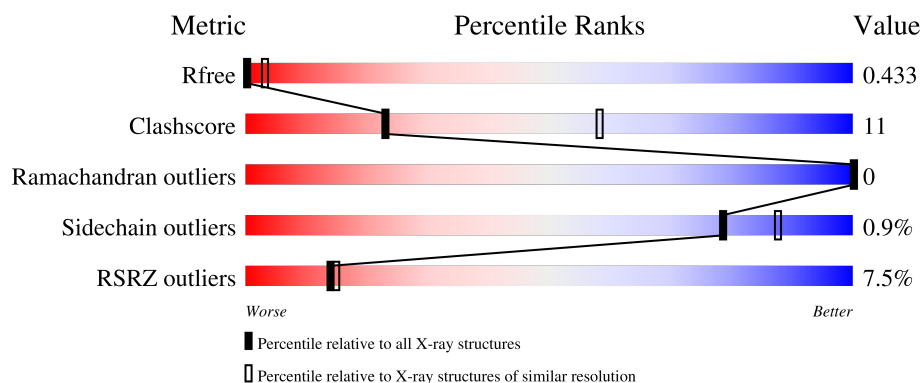
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 6.00 Å.

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




| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1000 (8.00-3.88)                                      |
| Clashscore            | 141614                      | 1049 (8.00-3.90)                                      |
| Ramachandran outliers | 138981                      | 1016 (8.00-3.86)                                      |
| Sidechain outliers    | 138945                      | 1017 (8.00-3.82)                                      |
| RSRZ outliers         | 127900                      | 1015 (8.20-3.78)                                      |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 446    | <div> <div>7%</div> <div>67%</div> <div>16%</div> <div>•</div> <div>16%</div> </div> |
| 1   | C     | 446    | <div> <div>5%</div> <div>66%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> |
| 2   | B     | 400    | <div> <div>44%</div> <div>•</div> <div>53%</div> </div>                              |
| 2   | D     | 400    | <div> <div>44%</div> <div>•</div> <div>53%</div> </div>                              |
| 3   | M     | 2300   | <div> <div>93%</div> <div>•</div> <div>•</div> </div>                                |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 3   | N     | 2300   | <br>93% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | KEG  | A     | 501 | -         | -        | X       | -                |
| 4   | KEG  | A     | 502 | -         | -        | X       | -                |
| 4   | KEG  | A     | 503 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-dependent RNA helicase SUB2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 374      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3010  | 1916 | 523 | 560 | 11 |         |         |       |
| 1   | C     | 374      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3010  | 1916 | 523 | 560 | 11 |         |         |       |

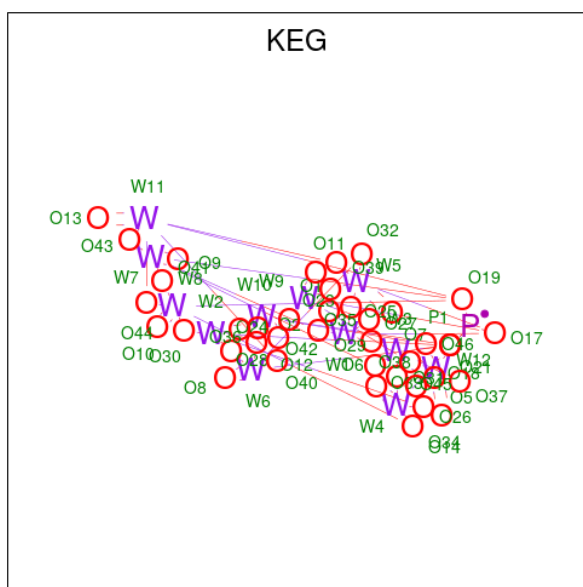
- Molecule 2 is a protein called Tex1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 2   | B     | 188      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 564 | 188 | 188 |         |         |       |
| 2   | D     | 188      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 564 | 188 | 188 |         |         |       |

- Molecule 3 is a protein called Tho2, Hpr1, Mft1, and Thp2.

| Mol | Chain | Residues | Atoms |      |      |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|---------|-------|
| 3   | M     | 2231     | Total | C    | N    | O    | 0       | 0       | 0     |
|     |       |          | 11155 | 6693 | 2231 | 2231 |         |         |       |
| 3   | N     | 2230     | Total | C    | N    | O    | 0       | 0       | 0     |
|     |       |          | 11150 | 6690 | 2230 | 2230 |         |         |       |

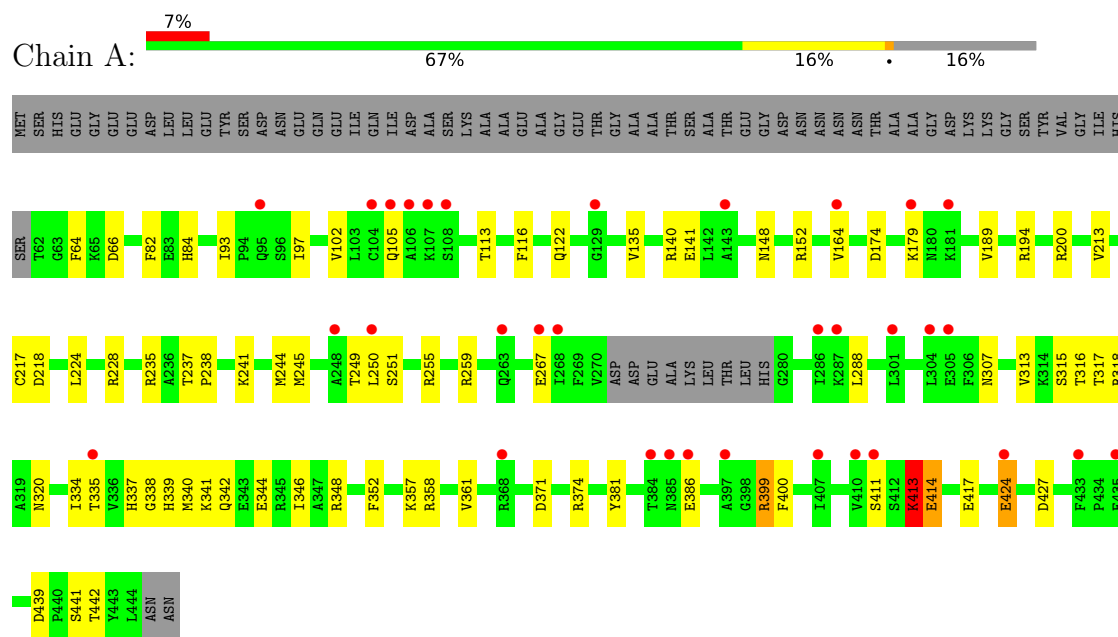
- Molecule 4 is 12-TUNGSTOPHOSPHATE (three-letter code: KEG) (formula: O<sub>40</sub>PW<sub>12</sub>).

[illegible]

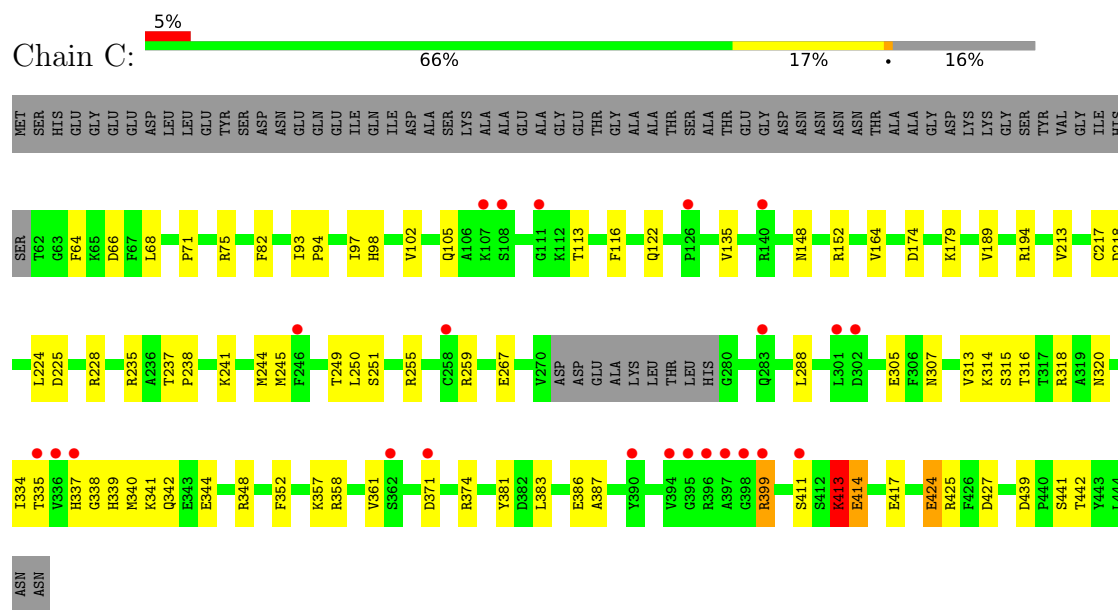
### 3 Residue-property plots

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

#### • Molecule 1: ATP-dependent RNA helicase SUB2



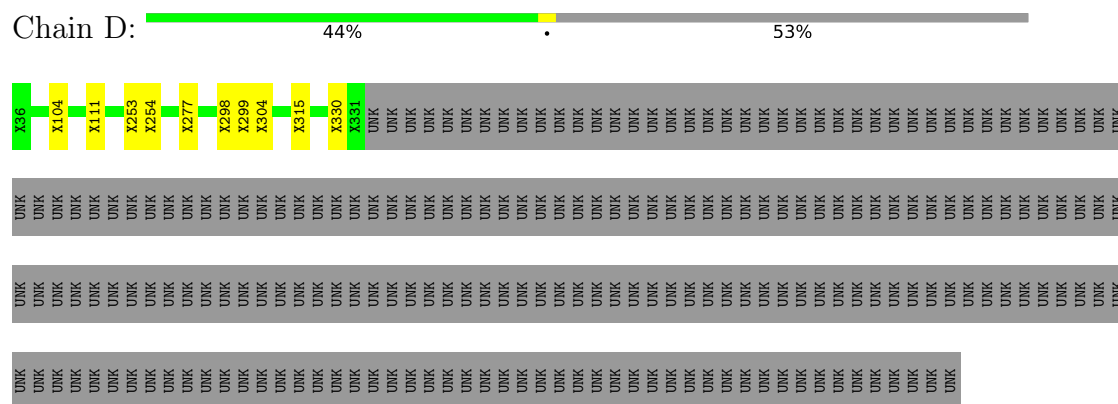
#### • Molecule 1: ATP-dependent RNA helicase SUB2



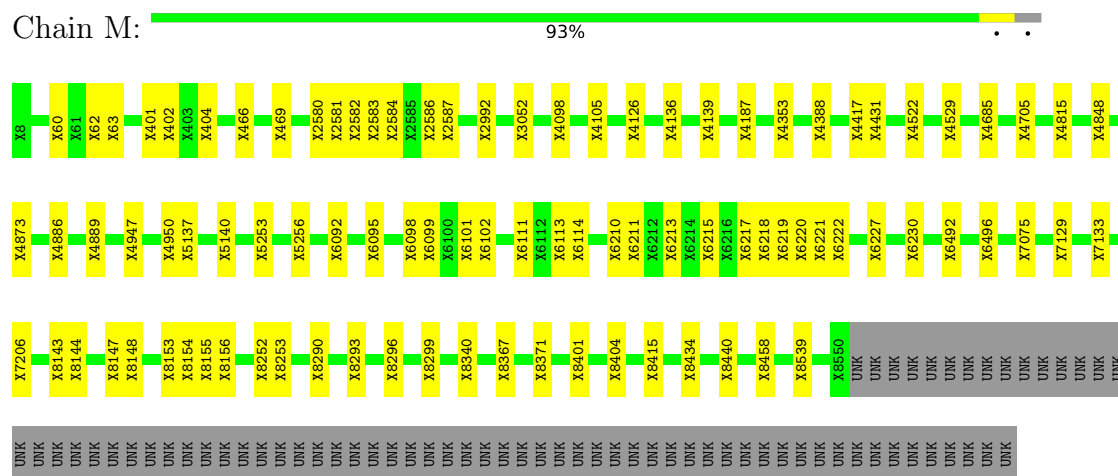
- Molecule 2: Tex1



- Molecule 2: Tex1



- Molecule 3: Tho2, Hpr1, Mft1, and Thp2



- Molecule 3: Tho2, Hpr1, Mft1, and Thp2



|     |       |       |       |     |
|-----|-------|-------|-------|-----|
| UNK | X9    | X4815 | X6492 | UNK |
| UNK | X60   | X4816 | X6496 | UNK |
| UNK | X61   | X4848 | UNK   | UNK |
| UNK | X62   | X4868 | X7075 | UNK |
| UNK | X63   | UNK   | UNK   | UNK |
| UNK | X401  | X4873 | X7129 | UNK |
| UNK | X402  | X4886 | X7133 | UNK |
| UNK | X403  | UNK   | UNK   | UNK |
| UNK | X404  | X4889 | X7206 | UNK |
| UNK | X466  | UNK   | UNK   | UNK |
| UNK | X469  | X4895 | X8119 | UNK |
| UNK | X2580 | UNK   | UNK   | UNK |
| UNK | X2581 | X4943 | X8143 | UNK |
| UNK | X2582 | UNK   | X8144 | UNK |
| UNK | X2583 | X4947 | UNK   | UNK |
| UNK | X2584 | UNK   | X8147 | UNK |
| UNK | X2585 | X4950 | X8148 | UNK |
| UNK | X2586 | X5137 | UNK   | UNK |
| UNK | X2587 | UNK   | X8153 | UNK |
| UNK | X2992 | X5140 | X8154 | UNK |
| UNK | X3052 | UNK   | X8155 | UNK |
| UNK | X4098 | X5253 | X8156 | UNK |
| UNK | X4105 | UNK   | UNK   | UNK |
| UNK | X4126 | X6092 | X8252 | UNK |
| UNK | X4136 | UNK   | X8253 | UNK |
| UNK | X4139 | X6095 | UNK   | UNK |
| UNK | X4187 | UNK   | X8290 | UNK |
| UNK | X4352 | X6098 | UNK   | UNK |
| UNK | X4388 | X6099 | X8293 | UNK |
| UNK | X4407 | X6100 | UNK   | UNK |
| UNK | X4417 | UNK   | X8296 | UNK |
| UNK | X4522 | X6101 | UNK   | UNK |
| UNK | X4529 | X6102 | UNK   | UNK |
| UNK | X4685 | UNK   | X8299 | UNK |
| UNK | X4695 | UNK   | UNK   | UNK |
| UNK | X4699 | X6111 | X8340 | UNK |
| UNK | X4705 | X6112 | UNK   | UNK |
|     |       | X6113 | UNK   | UNK |
|     |       | X6114 | X8367 | UNK |
|     |       | UNK   | UNK   | UNK |
|     |       | X6210 | X8371 | UNK |
|     |       | X6211 | UNK   | UNK |
|     |       | X6212 | X8401 | UNK |
|     |       | X6213 | UNK   | UNK |
|     |       | X6214 | X8404 | UNK |
|     |       | X6215 | UNK   | UNK |
|     |       | X6216 | X8415 | UNK |
|     |       | X6217 | UNK   | UNK |
|     |       | X6218 | X8434 | UNK |
|     |       | X6219 | UNK   | UNK |
|     |       | X6220 | UNK   | UNK |
|     |       | X6221 | X8440 | UNK |
|     |       | X6222 | UNK   | UNK |
|     |       | UNK   | X8458 | UNK |
|     |       | UNK   | UNK   | UNK |
|     |       | X6227 | X8539 | UNK |
|     |       | UNK   | UNK   | UNK |
|     |       | X6230 | X8550 | UNK |
|     |       | UNK   | UNK   | UNK |
|     |       | X6455 | UNK   | UNK |



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 153.34Å 319.53Å 176.44Å<br>90.00° 100.96° 90.00°            | Depositor        |
| Resolution (Å)  | 49.57 – 6.00<br>50.18 – 5.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (49.57-6.00)<br>96.9 (50.18-5.95)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.14  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.71 (at 6.15Å)   | Xtriage          |
| Refinement program  | PHENIX (1.10_2155)  | Depositor        |
| R, $R_{free}$   | 0.436 , 0.434<br>0.436 , 0.433                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2100 reflections (5.07%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 293.8   | Xtriage          |
| Anisotropy  | 0.512   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.18 , 320.5  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.74  | EDS              |
| Total number of atoms   | 30788   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 200.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KEG

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     | 0.41         | 1/3063 (0.0%) | 0.66        | 9/4131 (0.2%)  |
| 1   | C     | 0.41         | 1/3063 (0.0%) | 0.66        | 9/4131 (0.2%)  |
| All | All   | 0.41         | 2/6126 (0.0%) | 0.66        | 18/8262 (0.2%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 414 | GLU  | CD-OE1 | -5.23 | 1.19        | 1.25     |
| 1   | C     | 414 | GLU  | CD-OE1 | -5.22 | 1.20        | 1.25     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 427 | ASP  | CB-CA-C   | -8.73 | 92.94       | 110.40   |
| 1   | A     | 427 | ASP  | CB-CA-C   | -8.70 | 93.00       | 110.40   |
| 1   | C     | 427 | ASP  | CB-CG-OD2 | 8.41  | 125.87      | 118.30   |
| 1   | A     | 427 | ASP  | CB-CG-OD2 | 8.40  | 125.86      | 118.30   |
| 1   | A     | 427 | ASP  | CB-CG-OD1 | -7.39 | 111.65      | 118.30   |
| 1   | C     | 427 | ASP  | CB-CG-OD1 | -7.39 | 111.65      | 118.30   |
| 1   | A     | 417 | GLU  | CG-CD-OE2 | 6.71  | 131.72      | 118.30   |
| 1   | C     | 417 | GLU  | CG-CD-OE2 | 6.69  | 131.68      | 118.30   |
| 1   | C     | 414 | GLU  | CB-CA-C   | -6.69 | 97.02       | 110.40   |
| 1   | A     | 414 | GLU  | CB-CA-C   | -6.66 | 97.07       | 110.40   |
| 1   | A     | 424 | GLU  | CG-CD-OE1 | 6.46  | 131.22      | 118.30   |
| 1   | C     | 424 | GLU  | CG-CD-OE1 | 6.44  | 131.18      | 118.30   |
| 1   | C     | 427 | ASP  | N-CA-CB   | 6.07  | 121.53      | 110.60   |
| 1   | A     | 427 | ASP  | N-CA-CB   | 6.04  | 121.47      | 110.60   |
| 1   | C     | 417 | GLU  | CA-CB-CG  | 5.87  | 126.31      | 113.40   |
| 1   | A     | 417 | GLU  | CA-CB-CG  | 5.87  | 126.30      | 113.40   |
| 1   | C     | 413 | LYS  | CD-CE-NZ  | 5.43  | 124.20      | 111.70   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | A     | 413 | LYS  | CD-CE-NZ | 5.42 | 124.17      | 111.70   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3010  | 0        | 3043     | 158     | 0            |
| 1   | C     | 3010  | 0        | 3043     | 155     | 0            |
| 2   | B     | 940   | 0        | 262      | 6       | 0            |
| 2   | D     | 940   | 0        | 262      | 5       | 0            |
| 3   | M     | 11155 | 0        | 2489     | 100     | 0            |
| 3   | N     | 11150 | 0        | 2488     | 103     | 0            |
| 4   | A     | 159   | 0        | 0        | 53      | 0            |
| 4   | M     | 159   | 0        | 0        | 18      | 0            |
| 4   | N     | 265   | 0        | 0        | 30      | 0            |
| All | All   | 30788 | 0        | 11587    | 484     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (484) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:339:HIS:CB  | 1:C:341:LYS:CA  | 1.85                     | 1.53              |
| 1:A:339:HIS:CB  | 1:C:341:LYS:HA  | 1.36                     | 1.51              |
| 1:C:98:HIS:CG   | 3:N:4695:UNK:CB | 1.99                     | 1.45              |
| 1:A:316:THR:C   | 1:C:341:LYS:HZ2 | 1.14                     | 1.43              |
| 1:A:316:THR:C   | 1:C:341:LYS:NZ  | 1.70                     | 1.42              |
| 3:N:4815:UNK:CB | 3:N:4873:UNK:CB | 2.03                     | 1.36              |
| 1:A:339:HIS:HB3 | 1:C:341:LYS:CA  | 1.43                     | 1.36              |
| 3:M:4815:UNK:CB | 3:M:4873:UNK:CB | 2.02                     | 1.34              |
| 4:A:501:KEG:O45 | 1:C:341:LYS:HG2 | 1.19                     | 1.32              |
| 1:C:98:HIS:ND1  | 3:N:4695:UNK:CB | 1.85                     | 1.31              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:M:401:UNK:O   | 3:M:404:UNK:CB   | 1.83                     | 1.27              |
| 3:N:401:UNK:O   | 3:N:404:UNK:CB   | 1.83                     | 1.25              |
| 3:M:4098:UNK:CB | 3:M:4126:UNK:HA  | 1.69                     | 1.23              |
| 3:N:4098:UNK:CB | 3:N:4126:UNK:HA  | 1.69                     | 1.23              |
| 3:M:466:UNK:HA  | 3:M:5253:UNK:CB  | 1.69                     | 1.23              |
| 4:A:503:KEG:O10 | 1:C:314:LYS:O    | 1.54                     | 1.22              |
| 1:A:200:ARG:NH1 | 4:A:502:KEG:O2   | 1.72                     | 1.21              |
| 1:A:141:GLU:OE2 | 1:A:342:GLN:HG2  | 1.42                     | 1.20              |
| 4:A:501:KEG:O5  | 1:C:344:GLU:HG2  | 1.42                     | 1.20              |
| 2:D:277:UNK:CB  | 2:D:304:UNK:O    | 1.90                     | 1.20              |
| 1:A:340:MET:HA  | 4:A:501:KEG:O35  | 1.27                     | 1.19              |
| 2:B:277:UNK:CB  | 2:B:304:UNK:O    | 1.90                     | 1.18              |
| 1:A:340:MET:O   | 1:C:339:HIS:HA   | 1.40                     | 1.17              |
| 1:A:339:HIS:CG  | 1:C:341:LYS:CA   | 1.92                     | 1.17              |
| 1:C:71:PRO:HG2  | 3:N:4895:UNK:O   | 1.43                     | 1.16              |
| 4:A:501:KEG:O27 | 1:C:341:LYS:N    | 1.70                     | 1.16              |
| 1:A:339:HIS:CB  | 1:C:341:LYS:N    | 1.86                     | 1.16              |
| 4:A:502:KEG:O5  | 1:C:387:ALA:HB3  | 1.44                     | 1.16              |
| 1:A:141:GLU:HG2 | 1:A:342:GLN:HE21 | 1.11                     | 1.13              |
| 1:A:339:HIS:HB3 | 1:C:341:LYS:N    | 1.01                     | 1.11              |
| 1:A:342:GLN:HB2 | 1:C:339:HIS:CE1  | 1.85                     | 1.10              |
| 4:A:501:KEG:O5  | 1:C:344:GLU:CG   | 2.00                     | 1.10              |
| 4:A:503:KEG:O10 | 1:C:315:SER:CA   | 2.00                     | 1.10              |
| 1:A:339:HIS:HB2 | 1:C:341:LYS:HA   | 1.28                     | 1.09              |
| 1:A:342:GLN:CB  | 1:C:339:HIS:CE1  | 2.36                     | 1.09              |
| 3:M:6098:UNK:O  | 3:M:6101:UNK:CB  | 2.02                     | 1.08              |
| 3:N:6098:UNK:O  | 3:N:6101:UNK:CB  | 2.02                     | 1.08              |
| 3:N:4886:UNK:HA | 3:N:4950:UNK:C   | 1.84                     | 1.07              |
| 1:A:340:MET:CA  | 4:A:501:KEG:O35  | 2.01                     | 1.07              |
| 4:A:501:KEG:O45 | 1:C:341:LYS:CG   | 2.01                     | 1.07              |
| 3:M:4886:UNK:HA | 3:M:4950:UNK:C   | 1.84                     | 1.07              |
| 3:N:2992:UNK:O  | 3:N:3052:UNK:O   | 1.72                     | 1.06              |
| 1:C:413:LYS:HD2 | 1:C:414:GLU:H    | 1.19                     | 1.06              |
| 1:A:339:HIS:CG  | 1:C:341:LYS:HA   | 1.70                     | 1.06              |
| 3:M:2992:UNK:O  | 3:M:3052:UNK:O   | 1.72                     | 1.05              |
| 3:N:4886:UNK:CB | 3:N:4950:UNK:O   | 2.05                     | 1.05              |
| 1:A:413:LYS:HD2 | 1:A:414:GLU:H    | 1.19                     | 1.04              |
| 1:A:358:ARG:NH1 | 3:M:4353:UNK:HA  | 1.73                     | 1.04              |
| 3:M:4886:UNK:CB | 3:M:4950:UNK:O   | 2.05                     | 1.03              |
| 1:C:98:HIS:CD2  | 3:N:4695:UNK:CB  | 2.41                     | 1.03              |
| 3:N:6219:UNK:O  | 3:N:6222:UNK:N   | 1.93                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:358:ARG:NH1  | 3:M:4353:UNK:CA  | 2.21                     | 1.01              |
| 1:A:141:GLU:CG   | 1:A:342:GLN:HE21 | 1.73                     | 1.01              |
| 3:M:6219:UNK:O   | 3:M:6222:UNK:N   | 1.93                     | 1.01              |
| 4:A:503:KEG:O10  | 1:C:315:SER:HA   | 1.55                     | 1.00              |
| 3:N:8143:UNK:O   | 3:N:8147:UNK:N   | 1.94                     | 1.00              |
| 3:M:8143:UNK:O   | 3:M:8147:UNK:N   | 1.94                     | 0.99              |
| 1:A:340:MET:C    | 1:C:339:HIS:HA   | 1.83                     | 0.98              |
| 1:A:342:GLN:HB2  | 1:C:339:HIS:HE1  | 1.23                     | 0.98              |
| 3:N:7129:UNK:O   | 3:N:7133:UNK:N   | 1.98                     | 0.96              |
| 1:A:339:HIS:O    | 1:C:340:MET:CA   | 2.13                     | 0.96              |
| 1:C:75:ARG:HH12  | 3:N:4943:UNK:CB  | 1.79                     | 0.95              |
| 3:M:7129:UNK:O   | 3:M:7133:UNK:N   | 1.98                     | 0.94              |
| 3:M:4388:UNK:CB  | 3:M:4417:UNK:CB  | 2.46                     | 0.94              |
| 3:N:4388:UNK:CB  | 3:N:4417:UNK:CB  | 2.46                     | 0.93              |
| 3:M:466:UNK:CA   | 3:M:5253:UNK:CB  | 2.47                     | 0.93              |
| 1:A:358:ARG:HH11 | 3:M:4353:UNK:CA  | 1.82                     | 0.93              |
| 3:N:4886:UNK:CA  | 3:N:4950:UNK:C   | 2.46                     | 0.93              |
| 1:A:374:ARG:NE   | 3:M:4431:UNK:H2  | 1.67                     | 0.92              |
| 3:M:4886:UNK:CA  | 3:M:4950:UNK:C   | 2.46                     | 0.92              |
| 1:A:317:THR:N    | 1:C:341:LYS:NZ   | 2.17                     | 0.92              |
| 1:A:341:LYS:N    | 1:C:339:HIS:HB3  | 1.85                     | 0.91              |
| 3:N:466:UNK:HA   | 3:N:5253:UNK:CB  | 2.01                     | 0.91              |
| 3:M:8153:UNK:O   | 3:M:8156:UNK:CB  | 2.19                     | 0.90              |
| 4:A:503:KEG:O10  | 1:C:315:SER:CB   | 2.20                     | 0.90              |
| 1:A:337:HIS:CE1  | 1:C:341:LYS:HD3  | 2.06                     | 0.90              |
| 1:A:339:HIS:O    | 1:C:340:MET:HA   | 1.72                     | 0.90              |
| 3:N:8153:UNK:O   | 3:N:8156:UNK:CB  | 2.19                     | 0.90              |
| 1:A:340:MET:C    | 1:C:339:HIS:CA   | 2.39                     | 0.90              |
| 1:A:339:HIS:C    | 1:C:340:MET:N    | 2.27                     | 0.88              |
| 3:M:2583:UNK:O   | 3:M:2587:UNK:N   | 2.07                     | 0.88              |
| 3:M:4105:UNK:C   | 3:M:4187:UNK:O   | 2.22                     | 0.88              |
| 3:N:2583:UNK:O   | 3:N:2587:UNK:N   | 2.07                     | 0.87              |
| 3:N:4105:UNK:C   | 3:N:4187:UNK:O   | 2.22                     | 0.87              |
| 3:M:401:UNK:O    | 3:M:404:UNK:N    | 2.07                     | 0.87              |
| 1:A:316:THR:CB   | 1:C:341:LYS:NZ   | 2.37                     | 0.87              |
| 1:C:413:LYS:HD2  | 1:C:414:GLU:N    | 1.91                     | 0.86              |
| 1:A:316:THR:HB   | 1:C:341:LYS:CE   | 2.06                     | 0.85              |
| 1:A:340:MET:O    | 1:C:339:HIS:CA   | 2.24                     | 0.85              |
| 2:B:253:UNK:O    | 2:B:254:UNK:CB   | 2.25                     | 0.85              |
| 3:N:401:UNK:O    | 3:N:404:UNK:N    | 2.08                     | 0.85              |
| 1:A:141:GLU:CD   | 1:A:342:GLN:HG2  | 1.96                     | 0.84              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:337:HIS:HE1  | 4:A:501:KEG:O11 | 1.59                     | 0.84              |
| 1:A:235:ARG:HH12 | 3:M:6215:UNK:CB | 1.89                     | 0.84              |
| 3:M:4889:UNK:CB  | 3:M:4950:UNK:CB | 2.54                     | 0.84              |
| 3:N:4889:UNK:CB  | 3:N:4950:UNK:CB | 2.55                     | 0.84              |
| 1:A:141:GLU:OE2  | 1:A:342:GLN:CG  | 2.23                     | 0.84              |
| 2:D:253:UNK:O    | 2:D:254:UNK:CB  | 2.25                     | 0.84              |
| 1:A:140:ARG:HD2  | 4:A:503:KEG:O36 | 1.76                     | 0.84              |
| 1:A:337:HIS:CE1  | 4:A:501:KEG:O11 | 2.31                     | 0.83              |
| 1:A:413:LYS:HD2  | 1:A:414:GLU:N   | 1.91                     | 0.83              |
| 1:A:339:HIS:HE1  | 1:C:342:GLN:OE1 | 1.61                     | 0.82              |
| 3:N:4886:UNK:HA  | 3:N:4950:UNK:CB | 2.09                     | 0.82              |
| 3:M:8415:UNK:CB  | 3:M:8440:UNK:CB | 2.57                     | 0.82              |
| 3:M:4886:UNK:HA  | 3:M:4950:UNK:CB | 2.10                     | 0.81              |
| 3:M:6210:UNK:O   | 3:M:6213:UNK:N  | 2.13                     | 0.81              |
| 3:N:8415:UNK:CB  | 3:N:8440:UNK:CB | 2.57                     | 0.81              |
| 3:M:4522:UNK:CB  | 3:M:4529:UNK:N  | 2.43                     | 0.81              |
| 3:N:4522:UNK:CB  | 3:N:4529:UNK:N  | 2.43                     | 0.81              |
| 4:A:501:KEG:O11  | 1:C:341:LYS:HD3 | 1.81                     | 0.81              |
| 3:M:4886:UNK:CA  | 3:M:4950:UNK:O  | 2.29                     | 0.81              |
| 3:M:6111:UNK:O   | 3:M:6114:UNK:HA | 1.81                     | 0.80              |
| 3:N:6210:UNK:O   | 3:N:6213:UNK:N  | 2.13                     | 0.80              |
| 1:A:374:ARG:HE   | 3:M:4431:UNK:H2 | 1.29                     | 0.80              |
| 3:N:6111:UNK:O   | 3:N:6114:UNK:HA | 1.82                     | 0.79              |
| 3:N:8252:UNK:O   | 3:N:8253:UNK:C  | 2.30                     | 0.79              |
| 3:N:2580:UNK:O   | 3:N:2584:UNK:N  | 2.16                     | 0.79              |
| 1:A:84:HIS:HB2   | 1:A:400:PHE:HZ  | 1.47                     | 0.78              |
| 4:A:503:KEG:O10  | 1:C:314:LYS:C   | 2.20                     | 0.78              |
| 3:M:8252:UNK:O   | 3:M:8253:UNK:C  | 2.31                     | 0.78              |
| 3:N:4886:UNK:CA  | 3:N:4950:UNK:O  | 2.28                     | 0.78              |
| 1:A:316:THR:CA   | 1:C:341:LYS:NZ  | 2.47                     | 0.78              |
| 3:N:4889:UNK:CB  | 3:N:4947:UNK:HA | 2.14                     | 0.78              |
| 4:A:501:KEG:O1   | 1:C:341:LYS:N   | 2.15                     | 0.78              |
| 3:M:4889:UNK:CB  | 3:M:4947:UNK:HA | 2.14                     | 0.78              |
| 3:M:2580:UNK:O   | 3:M:2584:UNK:N  | 2.16                     | 0.78              |
| 1:C:358:ARG:NH1  | 3:N:4352:UNK:O  | 2.16                     | 0.77              |
| 1:A:200:ARG:NH1  | 4:A:502:KEG:O30 | 2.18                     | 0.76              |
| 1:A:341:LYS:N    | 1:C:339:HIS:CB  | 2.43                     | 0.76              |
| 1:A:141:GLU:HG2  | 1:A:342:GLN:NE2 | 1.96                     | 0.76              |
| 3:M:4886:UNK:CB  | 3:M:4950:UNK:C  | 2.64                     | 0.75              |
| 3:N:4098:UNK:CB  | 3:N:4126:UNK:CA | 2.59                     | 0.75              |
| 3:N:4886:UNK:CB  | 3:N:4950:UNK:C  | 2.64                     | 0.75              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:339:HIS:CE1  | 1:C:342:GLN:OE1 | 2.39                     | 0.75              |
| 3:N:4522:UNK:CB  | 3:N:4529:UNK:H2 | 2.00                     | 0.75              |
| 4:A:501:KEG:O5   | 1:C:344:GLU:CD  | 2.24                     | 0.75              |
| 3:M:4522:UNK:CB  | 3:M:4529:UNK:H2 | 2.00                     | 0.75              |
| 3:N:401:UNK:O    | 3:N:404:UNK:CA  | 2.35                     | 0.75              |
| 1:A:316:THR:HB   | 1:C:341:LYS:NZ  | 2.02                     | 0.74              |
| 3:M:401:UNK:O    | 3:M:404:UNK:CA  | 2.35                     | 0.74              |
| 3:M:466:UNK:CB   | 3:M:5253:UNK:CB | 2.66                     | 0.74              |
| 3:N:8144:UNK:HA  | 3:N:8147:UNK:CB | 2.18                     | 0.74              |
| 3:M:8144:UNK:HA  | 3:M:8147:UNK:CB | 2.18                     | 0.74              |
| 3:N:62:UNK:O     | 3:N:63:UNK:C    | 2.34                     | 0.74              |
| 1:A:358:ARG:HH12 | 3:M:4353:UNK:HA | 1.49                     | 0.74              |
| 3:M:62:UNK:O     | 3:M:63:UNK:C    | 2.34                     | 0.74              |
| 3:M:2582:UNK:O   | 3:M:2586:UNK:N  | 2.21                     | 0.73              |
| 1:C:71:PRO:HG2   | 3:N:4895:UNK:C  | 2.18                     | 0.73              |
| 1:A:339:HIS:C    | 1:C:340:MET:CA  | 2.53                     | 0.73              |
| 1:A:340:MET:O    | 1:C:339:HIS:CG  | 2.42                     | 0.72              |
| 3:N:6219:UNK:O   | 3:N:6220:UNK:C  | 2.36                     | 0.72              |
| 1:A:337:HIS:CE1  | 1:C:341:LYS:HE2 | 2.24                     | 0.72              |
| 3:N:2582:UNK:O   | 3:N:2586:UNK:N  | 2.21                     | 0.72              |
| 3:N:6219:UNK:C   | 3:N:6221:UNK:N  | 2.51                     | 0.71              |
| 3:M:4098:UNK:CB  | 3:M:4126:UNK:CA | 2.59                     | 0.71              |
| 1:C:66:ASP:OD1   | 3:N:4705:UNK:CB | 2.38                     | 0.71              |
| 1:A:84:HIS:HB2   | 1:A:400:PHE:CZ  | 2.26                     | 0.71              |
| 1:A:339:HIS:CG   | 1:C:341:LYS:N   | 2.43                     | 0.71              |
| 1:A:339:HIS:O    | 1:C:340:MET:C   | 2.29                     | 0.71              |
| 3:M:6219:UNK:O   | 3:M:6220:UNK:C  | 2.36                     | 0.71              |
| 1:A:340:MET:C    | 1:C:339:HIS:CB  | 2.59                     | 0.71              |
| 1:A:339:HIS:C    | 1:C:339:HIS:C   | 2.49                     | 0.71              |
| 1:A:337:HIS:HE1  | 1:C:341:LYS:HD3 | 1.53                     | 0.70              |
| 4:A:502:KEG:O5   | 1:C:387:ALA:CB  | 2.33                     | 0.70              |
| 4:A:503:KEG:O41  | 1:C:314:LYS:O   | 2.10                     | 0.69              |
| 3:N:8340:UNK:CB  | 3:N:8539:UNK:HA | 2.22                     | 0.69              |
| 1:A:316:THR:O    | 1:C:341:LYS:NZ  | 1.92                     | 0.69              |
| 3:M:8340:UNK:CB  | 3:M:8539:UNK:HA | 2.22                     | 0.68              |
| 1:A:374:ARG:CZ   | 3:M:4431:UNK:H2 | 2.05                     | 0.68              |
| 1:A:141:GLU:CD   | 1:A:342:GLN:CG  | 2.63                     | 0.68              |
| 1:C:94:PRO:HB3   | 3:N:4699:UNK:HA | 1.76                     | 0.68              |
| 3:N:6492:UNK:O   | 3:N:6496:UNK:CB | 2.42                     | 0.67              |
| 1:A:337:HIS:CE1  | 1:C:341:LYS:CD  | 2.79                     | 0.66              |
| 3:M:6219:UNK:C   | 3:M:6221:UNK:N  | 2.51                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:6492:UNK:O   | 3:M:6496:UNK:CB  | 2.42                     | 0.66              |
| 1:A:317:THR:N    | 1:C:341:LYS:HZ2  | 1.80                     | 0.66              |
| 1:C:75:ARG:NH1   | 3:N:4943:UNK:CB  | 2.56                     | 0.66              |
| 1:A:342:GLN:CA   | 1:C:339:HIS:CE1  | 2.55                     | 0.66              |
| 1:A:337:HIS:ND1  | 1:A:338:GLY:O    | 2.29                     | 0.66              |
| 1:A:341:LYS:HE2  | 1:C:316:THR:HB   | 1.77                     | 0.65              |
| 1:C:337:HIS:ND1  | 1:C:338:GLY:O    | 2.29                     | 0.65              |
| 1:A:340:MET:N    | 1:C:339:HIS:C    | 2.50                     | 0.65              |
| 1:C:439:ASP:OD2  | 1:C:441:SER:OG   | 2.15                     | 0.65              |
| 1:A:358:ARG:HH11 | 3:M:4353:UNK:C   | 2.10                     | 0.64              |
| 1:C:174:ASP:OD1  | 1:C:194:ARG:NH1  | 2.30                     | 0.64              |
| 1:A:174:ASP:OD1  | 1:A:194:ARG:NH1  | 2.30                     | 0.64              |
| 1:C:235:ARG:HH12 | 3:N:6215:UNK:CB  | 2.10                     | 0.64              |
| 1:A:341:LYS:HE2  | 1:C:316:THR:CB   | 2.28                     | 0.64              |
| 1:A:358:ARG:NH1  | 3:M:4353:UNK:N   | 2.17                     | 0.64              |
| 2:B:298:UNK:O    | 2:B:299:UNK:CB   | 2.46                     | 0.64              |
| 1:A:141:GLU:CG   | 1:A:342:GLN:NE2  | 2.56                     | 0.63              |
| 3:N:7129:UNK:O   | 3:N:7133:UNK:CB  | 2.47                     | 0.63              |
| 1:A:224:LEU:O    | 1:A:228:ARG:HG3  | 1.99                     | 0.63              |
| 3:M:7129:UNK:O   | 3:M:7133:UNK:CB  | 2.47                     | 0.63              |
| 1:A:316:THR:HB   | 1:C:341:LYS:CD   | 2.28                     | 0.62              |
| 1:A:339:HIS:HA   | 1:C:340:MET:N    | 2.14                     | 0.62              |
| 1:A:439:ASP:OD2  | 1:A:441:SER:OG   | 2.15                     | 0.62              |
| 4:A:502:KEG:O31  | 1:C:386:GLU:HG3  | 2.00                     | 0.62              |
| 1:C:237:THR:OG1  | 1:C:241:LYS:NZ   | 2.29                     | 0.62              |
| 1:C:224:LEU:O    | 1:C:228:ARG:HG3  | 1.99                     | 0.62              |
| 1:C:318:ARG:NH2  | 1:C:381:TYR:HE2  | 1.99                     | 0.61              |
| 3:N:8434:UNK:CB  | 3:N:8458:UNK:CB  | 2.79                     | 0.61              |
| 1:A:318:ARG:NH2  | 1:A:381:TYR:HE2  | 1.99                     | 0.60              |
| 3:N:8155:UNK:C   | 3:N:8156:UNK:O   | 2.49                     | 0.60              |
| 1:A:339:HIS:CA   | 1:C:340:MET:N    | 2.64                     | 0.60              |
| 3:M:8434:UNK:CB  | 3:M:8458:UNK:CB  | 2.79                     | 0.60              |
| 1:A:341:LYS:NZ   | 1:C:316:THR:OG1  | 2.34                     | 0.60              |
| 1:C:68:LEU:HD21  | 3:N:4868:UNK:CB  | 2.31                     | 0.60              |
| 3:M:2580:UNK:O   | 3:M:2584:UNK:CB  | 2.50                     | 0.60              |
| 1:A:337:HIS:CE1  | 1:C:341:LYS:CE   | 2.85                     | 0.60              |
| 2:D:298:UNK:O    | 2:D:299:UNK:CB   | 2.46                     | 0.60              |
| 3:M:8155:UNK:O   | 3:M:8156:UNK:C   | 2.49                     | 0.60              |
| 3:N:2580:UNK:O   | 3:N:2584:UNK:CB  | 2.50                     | 0.60              |
| 1:A:141:GLU:CD   | 1:A:342:GLN:HE21 | 2.05                     | 0.60              |
| 3:N:8155:UNK:O   | 3:N:8156:UNK:C   | 2.49                     | 0.59              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:340:MET:HA   | 1:C:339:HIS:O   | 2.01                     | 0.59              |
| 1:A:341:LYS:CD   | 1:C:339:HIS:CB  | 2.81                     | 0.58              |
| 3:M:6218:UNK:O   | 3:M:6221:UNK:CB | 2.51                     | 0.58              |
| 3:N:6218:UNK:O   | 3:N:6221:UNK:CB | 2.52                     | 0.58              |
| 3:M:8155:UNK:C   | 3:M:8156:UNK:O  | 2.49                     | 0.58              |
| 3:N:4685:UNK:CB  | 3:N:4848:UNK:HA | 2.35                     | 0.57              |
| 3:N:8367:UNK:CB  | 3:N:8404:UNK:O  | 2.53                     | 0.57              |
| 1:A:313:VAL:HG12 | 1:A:315:SER:H   | 1.70                     | 0.56              |
| 1:A:316:THR:HB   | 1:C:341:LYS:HD2 | 1.86                     | 0.56              |
| 1:A:340:MET:CA   | 1:C:339:HIS:O   | 2.53                     | 0.56              |
| 1:A:141:GLU:CD   | 1:A:342:GLN:NE2 | 2.59                     | 0.56              |
| 1:C:334:ILE:HG23 | 1:C:357:LYS:HD2 | 1.87                     | 0.56              |
| 3:M:4685:UNK:CB  | 3:M:4848:UNK:HA | 2.35                     | 0.56              |
| 1:A:339:HIS:HB3  | 4:A:501:KEG:O27 | 2.04                     | 0.56              |
| 1:C:313:VAL:HG12 | 1:C:315:SER:H   | 1.70                     | 0.56              |
| 3:M:6210:UNK:H   | 3:M:6213:UNK:CB | 2.19                     | 0.56              |
| 3:M:8367:UNK:CB  | 3:M:8404:UNK:O  | 2.53                     | 0.56              |
| 1:A:334:ILE:HG23 | 1:A:357:LYS:HD2 | 1.87                     | 0.56              |
| 3:N:4886:UNK:HA  | 3:N:4950:UNK:CA | 2.36                     | 0.56              |
| 3:N:6210:UNK:H   | 3:N:6213:UNK:CB | 2.19                     | 0.55              |
| 2:B:104:UNK:O    | 2:B:111:UNK:HA  | 2.06                     | 0.55              |
| 1:A:337:HIS:NE2  | 1:C:341:LYS:HE2 | 2.22                     | 0.55              |
| 1:A:341:LYS:CE   | 1:C:316:THR:OG1 | 2.55                     | 0.55              |
| 3:M:4886:UNK:HA  | 3:M:4950:UNK:CA | 2.36                     | 0.54              |
| 1:A:374:ARG:NE   | 3:M:4431:UNK:N  | 2.44                     | 0.54              |
| 2:D:104:UNK:O    | 2:D:111:UNK:HA  | 2.06                     | 0.54              |
| 3:N:6227:UNK:O   | 3:N:6230:UNK:CB | 2.56                     | 0.54              |
| 3:M:6227:UNK:O   | 3:M:6230:UNK:CB | 2.56                     | 0.53              |
| 4:A:502:KEG:O25  | 1:C:425:ARG:NE  | 2.35                     | 0.53              |
| 4:A:503:KEG:O10  | 1:C:315:SER:N   | 2.39                     | 0.53              |
| 3:M:60:UNK:O     | 3:M:63:UNK:CB   | 2.57                     | 0.53              |
| 3:M:6099:UNK:O   | 3:M:6102:UNK:N  | 2.42                     | 0.53              |
| 3:M:6210:UNK:O   | 3:M:6211:UNK:C  | 2.57                     | 0.53              |
| 1:A:339:HIS:CG   | 1:C:340:MET:C   | 2.30                     | 0.53              |
| 3:N:6210:UNK:O   | 3:N:6211:UNK:C  | 2.57                     | 0.53              |
| 1:A:342:GLN:CB   | 1:C:339:HIS:HE1 | 1.95                     | 0.52              |
| 4:A:501:KEG:O13  | 1:C:320:ASN:ND2 | 2.42                     | 0.52              |
| 1:A:386:GLU:OE2  | 1:C:225:ASP:OD2 | 2.27                     | 0.52              |
| 3:N:6219:UNK:O   | 3:N:6221:UNK:N  | 2.43                     | 0.52              |
| 1:A:316:THR:O    | 1:C:341:LYS:CE  | 2.58                     | 0.52              |
| 1:A:340:MET:HA   | 4:A:501:KEG:O32 | 2.10                     | 0.52              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:N:6455:UNK:CB | 3:N:8119:UNK:CB | 2.87                     | 0.52              |
| 3:M:5137:UNK:N  | 3:M:5140:UNK:CB | 2.73                     | 0.52              |
| 3:M:6219:UNK:O  | 3:M:6221:UNK:N  | 2.43                     | 0.52              |
| 3:N:6092:UNK:N  | 3:N:6095:UNK:CB | 2.73                     | 0.52              |
| 3:N:6099:UNK:O  | 3:N:6102:UNK:N  | 2.42                     | 0.52              |
| 1:A:413:LYS:CD  | 1:A:414:GLU:N   | 2.69                     | 0.52              |
| 1:C:344:GLU:O   | 1:C:348:ARG:HG3 | 2.10                     | 0.52              |
| 3:N:60:UNK:O    | 3:N:63:UNK:CB   | 2.57                     | 0.52              |
| 3:N:469:UNK:CB  | 3:N:5253:UNK:HA | 2.40                     | 0.52              |
| 3:N:5137:UNK:N  | 3:N:5140:UNK:CB | 2.73                     | 0.52              |
| 1:A:237:THR:OG1 | 1:A:241:LYS:NZ  | 2.29                     | 0.51              |
| 1:A:141:GLU:HG2 | 1:A:346:ILE:CG1 | 2.40                     | 0.51              |
| 1:A:344:GLU:O   | 1:A:348:ARG:HG3 | 2.10                     | 0.51              |
| 1:A:340:MET:CA  | 1:C:339:HIS:C   | 2.78                     | 0.51              |
| 1:A:341:LYS:HD2 | 1:C:339:HIS:CG  | 2.44                     | 0.51              |
| 3:M:469:UNK:CB  | 3:M:5256:UNK:CB | 2.88                     | 0.51              |
| 3:M:6092:UNK:N  | 3:M:6095:UNK:CB | 2.73                     | 0.51              |
| 1:A:255:ARG:O   | 1:A:259:ARG:HG3 | 2.10                     | 0.51              |
| 4:A:503:KEG:O10 | 1:C:315:SER:HB3 | 2.09                     | 0.51              |
| 1:C:255:ARG:O   | 1:C:259:ARG:HG3 | 2.10                     | 0.51              |
| 3:N:6099:UNK:C  | 3:N:6101:UNK:N  | 2.73                     | 0.50              |
| 1:C:413:LYS:CD  | 1:C:414:GLU:N   | 2.69                     | 0.50              |
| 3:M:62:UNK:O    | 3:M:63:UNK:O    | 2.30                     | 0.50              |
| 3:M:8290:UNK:O  | 3:M:8293:UNK:CB | 2.60                     | 0.50              |
| 3:M:8296:UNK:O  | 3:M:8299:UNK:O  | 2.30                     | 0.50              |
| 3:N:8340:UNK:CB | 3:N:8539:UNK:CA | 2.90                     | 0.50              |
| 3:M:8252:UNK:O  | 3:M:8253:UNK:O  | 2.30                     | 0.50              |
| 1:A:288:LEU:O   | 1:A:411:SER:HA  | 2.12                     | 0.50              |
| 3:N:8155:UNK:O  | 3:N:8156:UNK:O  | 2.30                     | 0.50              |
| 3:N:8371:UNK:CB | 3:N:8401:UNK:HA | 2.42                     | 0.50              |
| 1:C:71:PRO:CG   | 3:N:4895:UNK:O  | 2.37                     | 0.49              |
| 3:M:8155:UNK:O  | 3:M:8156:UNK:O  | 2.30                     | 0.49              |
| 1:A:340:MET:C   | 1:C:339:HIS:CG  | 2.81                     | 0.49              |
| 4:A:503:KEG:O34 | 1:C:315:SER:HA  | 2.11                     | 0.49              |
| 1:C:288:LEU:O   | 1:C:411:SER:HA  | 2.12                     | 0.49              |
| 3:M:8154:UNK:O  | 3:M:8156:UNK:O  | 2.30                     | 0.49              |
| 3:M:8371:UNK:CB | 3:M:8401:UNK:HA | 2.42                     | 0.49              |
| 1:C:305:GLU:OE1 | 3:N:4407:UNK:CB | 2.60                     | 0.49              |
| 3:N:62:UNK:O    | 3:N:63:UNK:O    | 2.30                     | 0.49              |
| 3:N:8252:UNK:O  | 3:N:8253:UNK:O  | 2.30                     | 0.49              |
| 3:N:8290:UNK:O  | 3:N:8293:UNK:CB | 2.60                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:8296:UNK:O   | 3:N:8299:UNK:O   | 2.30                     | 0.49              |
| 1:A:340:MET:O    | 1:C:339:HIS:CB   | 2.61                     | 0.49              |
| 3:N:8154:UNK:O   | 3:N:8156:UNK:O   | 2.30                     | 0.49              |
| 1:A:339:HIS:CD2  | 1:C:340:MET:C    | 2.78                     | 0.49              |
| 1:A:93:ILE:O     | 1:A:97:ILE:HG12  | 2.12                     | 0.49              |
| 3:M:469:UNK:CB   | 3:M:5253:UNK:HA  | 2.43                     | 0.49              |
| 3:N:4886:UNK:N   | 3:N:4950:UNK:O   | 2.46                     | 0.49              |
| 1:C:93:ILE:O     | 1:C:97:ILE:HG12  | 2.12                     | 0.48              |
| 1:A:358:ARG:HH11 | 3:M:4353:UNK:HA  | 1.50                     | 0.48              |
| 1:A:341:LYS:HD3  | 1:C:339:HIS:CB   | 2.43                     | 0.48              |
| 3:N:401:UNK:C    | 3:N:404:UNK:CB   | 2.83                     | 0.48              |
| 1:A:358:ARG:HH12 | 3:M:4353:UNK:CA  | 2.12                     | 0.48              |
| 1:A:316:THR:HB   | 1:C:341:LYS:HE2  | 1.95                     | 0.48              |
| 3:M:4136:UNK:O   | 3:M:4139:UNK:N   | 2.47                     | 0.48              |
| 3:N:7075:UNK:CB  | 3:N:7206:UNK:CB  | 2.92                     | 0.48              |
| 4:A:503:KEG:O41  | 4:A:503:KEG:O19  | 2.32                     | 0.48              |
| 4:N:8705:KEG:O41 | 4:N:8705:KEG:O19 | 2.32                     | 0.48              |
| 3:M:4886:UNK:N   | 3:M:4950:UNK:O   | 2.47                     | 0.47              |
| 1:C:164:VAL:HA   | 1:C:189:VAL:O    | 2.14                     | 0.47              |
| 4:M:8701:KEG:O41 | 4:M:8701:KEG:O19 | 2.32                     | 0.47              |
| 4:N:8701:KEG:O41 | 4:N:8701:KEG:O19 | 2.32                     | 0.47              |
| 4:A:501:KEG:O41  | 4:A:501:KEG:O19  | 2.32                     | 0.47              |
| 3:N:4136:UNK:O   | 3:N:4139:UNK:N   | 2.47                     | 0.47              |
| 4:N:8702:KEG:O41 | 4:N:8702:KEG:O19 | 2.32                     | 0.47              |
| 3:M:6098:UNK:O   | 3:M:6101:UNK:N   | 2.48                     | 0.47              |
| 3:M:7075:UNK:CB  | 3:M:7206:UNK:CB  | 2.92                     | 0.47              |
| 1:C:305:GLU:OE2  | 3:N:4407:UNK:CB  | 2.62                     | 0.47              |
| 1:A:341:LYS:HD3  | 1:C:339:HIS:HB2  | 1.96                     | 0.47              |
| 1:A:164:VAL:HA   | 1:A:189:VAL:O    | 2.14                     | 0.47              |
| 3:M:8340:UNK:CB  | 3:M:8539:UNK:CA  | 2.90                     | 0.47              |
| 4:N:8703:KEG:O41 | 4:N:8703:KEG:O19 | 2.33                     | 0.47              |
| 1:A:371:ASP:OD2  | 1:A:399:ARG:HD3  | 2.15                     | 0.47              |
| 1:C:439:ASP:HB3  | 1:C:442:THR:HG23 | 1.97                     | 0.47              |
| 4:M:8703:KEG:O17 | 4:M:8703:KEG:O35 | 2.33                     | 0.47              |
| 4:N:8704:KEG:O41 | 4:N:8704:KEG:O19 | 2.32                     | 0.47              |
| 4:A:501:KEG:O35  | 4:A:501:KEG:O17  | 2.33                     | 0.47              |
| 1:C:307:ASN:HB3  | 1:C:374:ARG:O    | 2.15                     | 0.47              |
| 4:M:8702:KEG:O41 | 4:M:8702:KEG:O19 | 2.32                     | 0.47              |
| 3:N:6098:UNK:O   | 3:N:6101:UNK:N   | 2.48                     | 0.47              |
| 4:M:8703:KEG:O41 | 4:M:8703:KEG:O19 | 2.32                     | 0.47              |
| 4:A:502:KEG:O43  | 4:A:502:KEG:O19  | 2.33                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:6112:UNK:HA  | 3:N:6113:UNK:HA  | 1.71                     | 0.46              |
| 1:A:307:ASN:HB3  | 1:A:374:ARG:O    | 2.16                     | 0.46              |
| 4:M:8701:KEG:O17 | 4:M:8701:KEG:O35 | 2.33                     | 0.46              |
| 4:N:8702:KEG:O19 | 4:N:8702:KEG:O43 | 2.34                     | 0.46              |
| 1:C:238:PRO:O    | 1:C:241:LYS:HD3  | 2.16                     | 0.46              |
| 4:A:501:KEG:O38  | 4:A:501:KEG:O21  | 2.34                     | 0.46              |
| 3:M:6099:UNK:C   | 3:M:6101:UNK:N   | 2.73                     | 0.46              |
| 4:M:8702:KEG:O17 | 4:M:8702:KEG:O35 | 2.33                     | 0.46              |
| 4:N:8702:KEG:O17 | 4:N:8702:KEG:O35 | 2.33                     | 0.46              |
| 4:A:501:KEG:O19  | 4:A:501:KEG:O43  | 2.34                     | 0.46              |
| 4:A:502:KEG:O19  | 4:A:502:KEG:O41  | 2.32                     | 0.46              |
| 3:M:8340:UNK:CB  | 3:M:8539:UNK:N   | 2.79                     | 0.46              |
| 4:M:8702:KEG:O19 | 4:M:8702:KEG:O43 | 2.33                     | 0.46              |
| 4:N:8701:KEG:O38 | 4:N:8701:KEG:O21 | 2.34                     | 0.46              |
| 4:M:8703:KEG:O19 | 4:M:8703:KEG:O43 | 2.33                     | 0.46              |
| 4:M:8703:KEG:O38 | 4:M:8703:KEG:O21 | 2.34                     | 0.46              |
| 4:N:8701:KEG:O19 | 4:N:8701:KEG:O43 | 2.34                     | 0.46              |
| 4:N:8702:KEG:O38 | 4:N:8702:KEG:O21 | 2.34                     | 0.46              |
| 4:M:8701:KEG:O21 | 4:M:8701:KEG:O38 | 2.34                     | 0.46              |
| 4:M:8702:KEG:O38 | 4:M:8702:KEG:O21 | 2.34                     | 0.46              |
| 3:N:8340:UNK:CB  | 3:N:8539:UNK:N   | 2.79                     | 0.46              |
| 1:A:341:LYS:CD   | 1:C:339:HIS:HB3  | 2.45                     | 0.46              |
| 4:N:8705:KEG:O19 | 4:N:8705:KEG:O43 | 2.34                     | 0.46              |
| 1:A:179:LYS:HE3  | 1:A:179:LYS:HB2  | 1.57                     | 0.46              |
| 3:M:402:UNK:C    | 3:M:404:UNK:N    | 2.76                     | 0.46              |
| 4:N:8703:KEG:O17 | 4:N:8703:KEG:O35 | 2.33                     | 0.46              |
| 4:N:8705:KEG:O38 | 4:N:8705:KEG:O21 | 2.34                     | 0.46              |
| 1:A:339:HIS:HA   | 1:C:340:MET:H    | 1.81                     | 0.46              |
| 4:A:502:KEG:O17  | 4:A:502:KEG:O35  | 2.33                     | 0.46              |
| 4:N:8704:KEG:O19 | 4:N:8704:KEG:O43 | 2.33                     | 0.46              |
| 1:A:374:ARG:NH2  | 3:M:4431:UNK:H2  | 2.14                     | 0.45              |
| 1:C:371:ASP:OD2  | 1:C:399:ARG:HD3  | 2.15                     | 0.45              |
| 4:N:8704:KEG:O17 | 4:N:8704:KEG:O35 | 2.33                     | 0.45              |
| 1:C:383:LEU:HD12 | 1:C:383:LEU:HA   | 1.85                     | 0.45              |
| 4:N:8703:KEG:O38 | 4:N:8703:KEG:O21 | 2.34                     | 0.45              |
| 4:N:8705:KEG:O17 | 4:N:8705:KEG:O35 | 2.33                     | 0.45              |
| 1:A:238:PRO:O    | 1:A:241:LYS:HD3  | 2.15                     | 0.45              |
| 4:A:502:KEG:O38  | 4:A:502:KEG:O21  | 2.34                     | 0.45              |
| 3:N:466:UNK:CA   | 3:N:5253:UNK:CB  | 2.86                     | 0.45              |
| 4:A:503:KEG:O17  | 4:A:503:KEG:O35  | 2.33                     | 0.45              |
| 4:M:8701:KEG:O19 | 4:M:8701:KEG:O43 | 2.33                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:401:UNK:C    | 3:N:404:UNK:N    | 2.79                     | 0.45              |
| 4:N:8701:KEG:O17 | 4:N:8701:KEG:O35 | 2.33                     | 0.45              |
| 4:N:8703:KEG:O19 | 4:N:8703:KEG:O43 | 2.33                     | 0.45              |
| 1:A:64:PHE:CE2   | 1:A:82:PHE:HB3   | 2.51                     | 0.45              |
| 1:A:439:ASP:HB3  | 1:A:442:THR:HG23 | 1.97                     | 0.45              |
| 4:A:503:KEG:O21  | 4:A:503:KEG:O38  | 2.34                     | 0.45              |
| 1:C:64:PHE:CE2   | 1:C:82:PHE:HB3   | 2.51                     | 0.45              |
| 3:N:402:UNK:C    | 3:N:404:UNK:N    | 2.75                     | 0.45              |
| 4:A:503:KEG:O19  | 4:A:503:KEG:O43  | 2.34                     | 0.45              |
| 1:C:251:SER:O    | 1:C:255:ARG:HG3  | 2.16                     | 0.45              |
| 4:N:8704:KEG:O38 | 4:N:8704:KEG:O21 | 2.34                     | 0.45              |
| 3:M:401:UNK:C    | 3:M:404:UNK:N    | 2.78                     | 0.45              |
| 3:M:6113:UNK:CB  | 3:M:6114:UNK:CB  | 2.95                     | 0.45              |
| 1:A:141:GLU:HB3  | 1:A:346:ILE:HD11 | 1.98                     | 0.45              |
| 1:A:251:SER:O    | 1:A:255:ARG:HG3  | 2.16                     | 0.45              |
| 1:A:339:HIS:O    | 1:C:341:LYS:N    | 2.48                     | 0.45              |
| 3:N:6113:UNK:CB  | 3:N:6114:UNK:CB  | 2.95                     | 0.45              |
| 1:A:340:MET:C    | 4:A:501:KEG:O7   | 2.56                     | 0.44              |
| 1:A:66:ASP:HB3   | 3:M:4705:UNK:CB  | 2.47                     | 0.44              |
| 1:C:179:LYS:HB2  | 1:C:179:LYS:HE3  | 1.57                     | 0.44              |
| 3:M:6217:UNK:O   | 3:M:6220:UNK:CB  | 2.66                     | 0.44              |
| 3:N:4886:UNK:CA  | 3:N:4950:UNK:CB  | 2.91                     | 0.44              |
| 1:A:341:LYS:HE2  | 1:C:316:THR:OG1  | 2.18                     | 0.44              |
| 1:A:341:LYS:HD2  | 1:C:339:HIS:CB   | 2.47                     | 0.44              |
| 1:A:342:GLN:CB   | 1:C:339:HIS:NE2  | 2.39                     | 0.44              |
| 1:C:97:ILE:HD12  | 1:C:122:GLN:HG2  | 1.99                     | 0.44              |
| 3:N:2582:UNK:O   | 3:N:2586:UNK:CB  | 2.65                     | 0.44              |
| 1:A:97:ILE:HD12  | 1:A:122:GLN:HG2  | 1.99                     | 0.44              |
| 3:M:401:UNK:C    | 3:M:404:UNK:CB   | 2.83                     | 0.44              |
| 3:M:2582:UNK:O   | 3:M:2586:UNK:CB  | 2.65                     | 0.44              |
| 3:M:6492:UNK:O   | 3:M:6496:UNK:N   | 2.51                     | 0.44              |
| 4:N:8702:KEG:O21 | 4:N:8702:KEG:O37 | 2.36                     | 0.44              |
| 1:C:334:ILE:HD11 | 1:C:352:PHE:HB2  | 2.00                     | 0.44              |
| 3:N:6492:UNK:O   | 3:N:6496:UNK:N   | 2.51                     | 0.44              |
| 4:A:502:KEG:O19  | 4:A:502:KEG:O44  | 2.37                     | 0.43              |
| 4:N:8701:KEG:O21 | 4:N:8701:KEG:O37 | 2.37                     | 0.43              |
| 1:A:320:ASN:ND2  | 1:C:341:LYS:HE3  | 2.34                     | 0.43              |
| 4:N:8704:KEG:O19 | 4:N:8704:KEG:O44 | 2.37                     | 0.43              |
| 4:A:501:KEG:O21  | 4:A:501:KEG:O37  | 2.36                     | 0.43              |
| 4:M:8703:KEG:O21 | 4:M:8703:KEG:O37 | 2.36                     | 0.43              |
| 3:N:8144:UNK:O   | 3:N:8148:UNK:N   | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:N:8701:KEG:O19 | 4:N:8701:KEG:O44 | 2.37                     | 0.43              |
| 1:A:102:VAL:HB   | 1:A:244:MET:HG2  | 2.00                     | 0.43              |
| 4:M:8702:KEG:O21 | 4:M:8702:KEG:O37 | 2.36                     | 0.43              |
| 4:N:8704:KEG:O21 | 4:N:8704:KEG:O37 | 2.36                     | 0.43              |
| 4:N:8705:KEG:O19 | 4:N:8705:KEG:O44 | 2.37                     | 0.43              |
| 4:A:501:KEG:O19  | 4:A:501:KEG:O44  | 2.37                     | 0.43              |
| 4:N:8705:KEG:O21 | 4:N:8705:KEG:O37 | 2.36                     | 0.43              |
| 1:A:135:VAL:HG22 | 1:A:213:VAL:HB   | 2.01                     | 0.43              |
| 4:A:502:KEG:O21  | 4:A:502:KEG:O37  | 2.37                     | 0.43              |
| 3:N:6217:UNK:O   | 3:N:6220:UNK:CB  | 2.66                     | 0.43              |
| 3:N:7129:UNK:O   | 3:N:7133:UNK:CA  | 2.66                     | 0.43              |
| 3:M:7129:UNK:O   | 3:M:7133:UNK:CA  | 2.66                     | 0.42              |
| 3:M:8144:UNK:O   | 3:M:8148:UNK:N   | 2.52                     | 0.42              |
| 1:A:113:THR:HA   | 1:A:116:PHE:CE2  | 2.53                     | 0.42              |
| 1:A:341:LYS:HD2  | 1:C:339:HIS:CD2  | 2.54                     | 0.42              |
| 4:A:503:KEG:O21  | 4:A:503:KEG:O37  | 2.37                     | 0.42              |
| 4:N:8703:KEG:O21 | 4:N:8703:KEG:O37 | 2.36                     | 0.42              |
| 4:M:8701:KEG:O19 | 4:M:8701:KEG:O44 | 2.37                     | 0.42              |
| 4:M:8701:KEG:O21 | 4:M:8701:KEG:O37 | 2.37                     | 0.42              |
| 4:M:8702:KEG:O19 | 4:M:8702:KEG:O44 | 2.37                     | 0.42              |
| 4:M:8703:KEG:O19 | 4:M:8703:KEG:O44 | 2.36                     | 0.42              |
| 2:B:277:UNK:CB   | 2:B:304:UNK:C    | 2.86                     | 0.42              |
| 1:C:113:THR:HA   | 1:C:116:PHE:CE2  | 2.54                     | 0.42              |
| 1:A:141:GLU:CG   | 1:A:346:ILE:HG13 | 2.49                     | 0.42              |
| 4:N:8702:KEG:O19 | 4:N:8702:KEG:O44 | 2.37                     | 0.42              |
| 1:A:341:LYS:N    | 4:A:501:KEG:O32  | 2.47                     | 0.42              |
| 4:A:503:KEG:O19  | 4:A:503:KEG:O44  | 2.37                     | 0.42              |
| 4:N:8703:KEG:O19 | 4:N:8703:KEG:O44 | 2.37                     | 0.42              |
| 1:A:141:GLU:HG3  | 1:A:346:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:334:ILE:HD11 | 1:A:352:PHE:HB2  | 2.00                     | 0.42              |
| 1:C:102:VAL:HB   | 1:C:244:MET:HG2  | 2.00                     | 0.42              |
| 1:C:135:VAL:HG22 | 1:C:213:VAL:HB   | 2.01                     | 0.42              |
| 3:N:2581:UNK:HA  | 3:N:2584:UNK:CB  | 2.50                     | 0.42              |
| 1:A:313:VAL:HG11 | 1:A:318:ARG:HB2  | 2.02                     | 0.42              |
| 4:A:502:KEG:O6   | 1:C:386:GLU:HA   | 2.19                     | 0.42              |
| 1:C:105:GLN:HB2  | 1:C:250:LEU:HD12 | 2.02                     | 0.41              |
| 3:N:62:UNK:C     | 3:N:63:UNK:O     | 2.65                     | 0.41              |
| 1:A:235:ARG:NH1  | 3:M:6215:UNK:CB  | 2.70                     | 0.41              |
| 1:C:218:ASP:OD2  | 1:C:249:THR:OG1  | 2.38                     | 0.41              |
| 3:M:2581:UNK:HA  | 3:M:2584:UNK:CB  | 2.50                     | 0.41              |
| 1:A:105:GLN:HB2  | 1:A:250:LEU:HD12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:259:ARG:NH1  | 1:A:267:GLU:OE1 | 2.53                     | 0.41              |
| 1:C:148:ASN:O    | 1:C:152:ARG:HG3 | 2.20                     | 0.41              |
| 3:N:6098:UNK:O   | 3:N:6101:UNK:CA | 2.67                     | 0.41              |
| 1:A:313:VAL:CG1  | 1:A:318:ARG:HB2 | 2.51                     | 0.41              |
| 1:A:341:LYS:CD   | 1:C:339:HIS:HB2 | 2.49                     | 0.41              |
| 1:C:313:VAL:HG11 | 1:C:318:ARG:HB2 | 2.02                     | 0.41              |
| 1:A:148:ASN:O    | 1:A:152:ARG:HG3 | 2.20                     | 0.41              |
| 1:C:316:THR:HG22 | 1:C:337:HIS:HB2 | 2.02                     | 0.41              |
| 1:A:316:THR:HG22 | 1:A:337:HIS:HB2 | 2.02                     | 0.41              |
| 1:A:316:THR:OG1  | 1:C:341:LYS:NZ  | 2.54                     | 0.41              |
| 1:A:335:THR:HA   | 1:A:361:VAL:O   | 2.21                     | 0.41              |
| 4:A:501:KEG:O27  | 1:C:341:LYS:HG2 | 2.20                     | 0.41              |
| 1:C:259:ARG:NH1  | 1:C:267:GLU:OE1 | 2.53                     | 0.41              |
| 3:N:6092:UNK:N   | 3:N:6095:UNK:N  | 2.60                     | 0.41              |
| 1:C:313:VAL:CG1  | 1:C:318:ARG:HB2 | 2.51                     | 0.41              |
| 1:A:218:ASP:OD2  | 1:A:249:THR:OG1 | 2.38                     | 0.40              |
| 2:B:315:UNK:HA   | 2:B:330:UNK:O   | 2.22                     | 0.40              |
| 1:C:335:THR:HA   | 1:C:361:VAL:O   | 2.21                     | 0.40              |
| 2:D:315:UNK:HA   | 2:D:330:UNK:O   | 2.22                     | 0.40              |
| 1:C:217:CYS:SG   | 1:C:245:MET:HB3 | 2.62                     | 0.40              |
| 3:N:6099:UNK:O   | 3:N:6102:UNK:CB | 2.69                     | 0.40              |
| 1:A:217:CYS:SG   | 1:A:245:MET:HB3 | 2.61                     | 0.40              |
| 3:M:6099:UNK:O   | 3:M:6102:UNK:CB | 2.69                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 370/446 (83%) | 362 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | C     | 370/446 (83%) | 362 (98%) | 8 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| All | All   | 740/892 (83%) | 724 (98%) | 16 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 331/386 (86%) | 328 (99%) | 3 (1%)   | 78          | 88 |
| 1   | C     | 331/386 (86%) | 328 (99%) | 3 (1%)   | 78          | 88 |
| All | All   | 662/772 (86%) | 656 (99%) | 6 (1%)   | 78          | 88 |

All (6) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 399 | ARG  |
| 1   | A     | 413 | LYS  |
| 1   | A     | 424 | GLU  |
| 1   | C     | 399 | ARG  |
| 1   | C     | 413 | LYS  |
| 1   | C     | 424 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 299 | GLN  |
| 1   | A     | 342 | GLN  |
| 1   | C     | 98  | HIS  |
| 1   | C     | 299 | GLN  |
| 1   | C     | 339 | HIS  |



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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 | $\# Z  > 2$ |
| 4   | KEG  | N     | 8704 | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.38 | 2 (33%)     |
| 4   | KEG  | A     | 503  | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.37 | 2 (33%)     |
| 4   | KEG  | A     | 501  | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.37 | 2 (33%)     |
| 4   | KEG  | N     | 8703 | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.38 | 2 (33%)     |
| 4   | KEG  | A     | 502  | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.38 | 2 (33%)     |
| 4   | KEG  | M     | 8703 | -    | 76,76,76     | 3.16 | 43 (56%)    | 6,234,234   | 1.39 | 2 (33%)     |
| 4   | KEG  | N     | 8702 | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.38 | 2 (33%)     |
| 4   | KEG  | M     | 8702 | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.37 | 2 (33%)     |
| 4   | KEG  | M     | 8701 | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.40 | 2 (33%)     |
| 4   | KEG  | N     | 8705 | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.39 | 2 (33%)     |
| 4   | KEG  | N     | 8701 | -    | 76,76,76     | 3.16 | 42 (55%)    | 6,234,234   | 1.37 | 2 (33%)     |

All (463) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | N     | 8704 | KEG  | P1-O18 | -7.90 | 1.27        | 1.54     |
| 4   | A     | 503  | KEG  | P1-O18 | -7.89 | 1.27        | 1.54     |
| 4   | M     | 8701 | KEG  | P1-O18 | -7.89 | 1.27        | 1.54     |
| 4   | N     | 8701 | KEG  | P1-O18 | -7.88 | 1.27        | 1.54     |
| 4   | A     | 501  | KEG  | P1-O18 | -7.88 | 1.27        | 1.54     |
| 4   | M     | 8702 | KEG  | P1-O18 | -7.88 | 1.27        | 1.54     |
| 4   | A     | 502  | KEG  | P1-O18 | -7.87 | 1.27        | 1.54     |
| 4   | N     | 8705 | KEG  | P1-O18 | -7.87 | 1.27        | 1.54     |
| 4   | N     | 8703 | KEG  | P1-O18 | -7.87 | 1.27        | 1.54     |
| 4   | M     | 8703 | KEG  | P1-O18 | -7.86 | 1.27        | 1.54     |
| 4   | N     | 8702 | KEG  | P1-O18 | -7.84 | 1.27        | 1.54     |
| 4   | M     | 8702 | KEG  | W2-O28 | -7.79 | 1.55        | 1.93     |
| 4   | N     | 8704 | KEG  | W2-O28 | -7.76 | 1.55        | 1.93     |
| 4   | A     | 503  | KEG  | W2-O28 | -7.75 | 1.55        | 1.93     |
| 4   | M     | 8703 | KEG  | W2-O28 | -7.75 | 1.55        | 1.93     |
| 4   | M     | 8701 | KEG  | W2-O28 | -7.75 | 1.55        | 1.93     |
| 4   | N     | 8705 | KEG  | W2-O28 | -7.75 | 1.55        | 1.93     |
| 4   | A     | 501  | KEG  | W2-O28 | -7.75 | 1.55        | 1.93     |
| 4   | N     | 8701 | KEG  | W2-O28 | -7.75 | 1.55        | 1.93     |
| 4   | N     | 8702 | KEG  | W2-O28 | -7.74 | 1.55        | 1.93     |
| 4   | A     | 502  | KEG  | W2-O28 | -7.74 | 1.55        | 1.93     |
| 4   | N     | 8703 | KEG  | W2-O28 | -7.73 | 1.55        | 1.93     |
| 4   | A     | 501  | KEG  | W6-O36 | -7.27 | 1.58        | 1.93     |
| 4   | M     | 8701 | KEG  | W6-O36 | -7.25 | 1.58        | 1.93     |
| 4   | M     | 8702 | KEG  | W6-O36 | -7.25 | 1.58        | 1.93     |
| 4   | A     | 503  | KEG  | W6-O36 | -7.25 | 1.58        | 1.93     |
| 4   | N     | 8705 | KEG  | W6-O36 | -7.25 | 1.58        | 1.93     |
| 4   | N     | 8701 | KEG  | W6-O36 | -7.25 | 1.58        | 1.93     |
| 4   | M     | 8703 | KEG  | W6-O36 | -7.24 | 1.58        | 1.93     |
| 4   | N     | 8703 | KEG  | W6-O36 | -7.24 | 1.58        | 1.93     |
| 4   | A     | 502  | KEG  | W6-O36 | -7.24 | 1.58        | 1.93     |
| 4   | N     | 8704 | KEG  | W6-O36 | -7.23 | 1.58        | 1.93     |
| 4   | N     | 8702 | KEG  | W6-O36 | -7.23 | 1.58        | 1.93     |
| 4   | N     | 8704 | KEG  | W1-O29 | -7.11 | 1.60        | 1.91     |
| 4   | A     | 502  | KEG  | W1-O29 | -7.11 | 1.60        | 1.91     |
| 4   | N     | 8702 | KEG  | W1-O29 | -7.10 | 1.60        | 1.91     |
| 4   | N     | 8701 | KEG  | W1-O29 | -7.10 | 1.60        | 1.91     |
| 4   | M     | 8703 | KEG  | W1-O29 | -7.10 | 1.60        | 1.91     |
| 4   | M     | 8702 | KEG  | W1-O29 | -7.10 | 1.60        | 1.91     |
| 4   | M     | 8701 | KEG  | W1-O29 | -7.10 | 1.60        | 1.91     |
| 4   | A     | 503  | KEG  | W1-O29 | -7.10 | 1.60        | 1.91     |
| 4   | A     | 501  | KEG  | W1-O29 | -7.09 | 1.60        | 1.91     |
| 4   | N     | 8703 | KEG  | W1-O29 | -7.08 | 1.60        | 1.91     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | N     | 8705 | KEG  | W1-O29  | -7.08 | 1.60        | 1.91     |
| 4   | A     | 502  | KEG  | W3-O33  | -7.00 | 1.61        | 1.91     |
| 4   | M     | 8702 | KEG  | W3-O33  | -6.98 | 1.61        | 1.91     |
| 4   | A     | 501  | KEG  | W3-O33  | -6.98 | 1.61        | 1.91     |
| 4   | M     | 8701 | KEG  | W3-O33  | -6.98 | 1.61        | 1.91     |
| 4   | N     | 8703 | KEG  | W3-O33  | -6.97 | 1.61        | 1.91     |
| 4   | A     | 503  | KEG  | W3-O33  | -6.96 | 1.61        | 1.91     |
| 4   | N     | 8701 | KEG  | W3-O33  | -6.96 | 1.61        | 1.91     |
| 4   | M     | 8703 | KEG  | W3-O33  | -6.95 | 1.61        | 1.91     |
| 4   | N     | 8705 | KEG  | W3-O33  | -6.95 | 1.61        | 1.91     |
| 4   | N     | 8704 | KEG  | W3-O33  | -6.95 | 1.61        | 1.91     |
| 4   | N     | 8702 | KEG  | W3-O33  | -6.94 | 1.61        | 1.91     |
| 4   | N     | 8703 | KEG  | W10-O28 | -5.64 | 1.66        | 1.93     |
| 4   | A     | 501  | KEG  | W10-O28 | -5.63 | 1.66        | 1.93     |
| 4   | A     | 502  | KEG  | W10-O28 | -5.63 | 1.66        | 1.93     |
| 4   | N     | 8701 | KEG  | W10-O28 | -5.63 | 1.66        | 1.93     |
| 4   | M     | 8703 | KEG  | W10-O28 | -5.63 | 1.66        | 1.93     |
| 4   | M     | 8702 | KEG  | W10-O28 | -5.63 | 1.66        | 1.93     |
| 4   | N     | 8702 | KEG  | W10-O28 | -5.63 | 1.66        | 1.93     |
| 4   | M     | 8701 | KEG  | W10-O28 | -5.62 | 1.66        | 1.93     |
| 4   | N     | 8705 | KEG  | W10-O28 | -5.62 | 1.66        | 1.93     |
| 4   | A     | 503  | KEG  | W10-O28 | -5.62 | 1.66        | 1.93     |
| 4   | N     | 8704 | KEG  | W10-O28 | -5.61 | 1.66        | 1.93     |
| 4   | A     | 502  | KEG  | W5-O23  | -5.22 | 1.68        | 1.93     |
| 4   | M     | 8703 | KEG  | W5-O23  | -5.21 | 1.68        | 1.93     |
| 4   | A     | 503  | KEG  | W5-O23  | -5.20 | 1.68        | 1.93     |
| 4   | A     | 501  | KEG  | W5-O23  | -5.20 | 1.68        | 1.93     |
| 4   | M     | 8701 | KEG  | W5-O23  | -5.20 | 1.68        | 1.93     |
| 4   | M     | 8702 | KEG  | W5-O23  | -5.19 | 1.68        | 1.93     |
| 4   | N     | 8703 | KEG  | W5-O23  | -5.19 | 1.68        | 1.93     |
| 4   | N     | 8701 | KEG  | W5-O23  | -5.19 | 1.68        | 1.93     |
| 4   | N     | 8705 | KEG  | W5-O23  | -5.19 | 1.68        | 1.93     |
| 4   | N     | 8702 | KEG  | W5-O23  | -5.19 | 1.68        | 1.93     |
| 4   | N     | 8704 | KEG  | W5-O23  | -5.17 | 1.68        | 1.93     |
| 4   | N     | 8703 | KEG  | P1-O19  | -4.75 | 1.38        | 1.54     |
| 4   | M     | 8702 | KEG  | W7-O29  | -4.75 | 1.70        | 1.91     |
| 4   | N     | 8705 | KEG  | W7-O29  | -4.75 | 1.70        | 1.91     |
| 4   | A     | 503  | KEG  | W7-O29  | -4.75 | 1.70        | 1.91     |
| 4   | M     | 8701 | KEG  | W7-O29  | -4.75 | 1.70        | 1.91     |
| 4   | N     | 8704 | KEG  | W7-O29  | -4.74 | 1.70        | 1.91     |
| 4   | A     | 501  | KEG  | W7-O29  | -4.74 | 1.70        | 1.91     |
| 4   | A     | 502  | KEG  | W7-O29  | -4.74 | 1.70        | 1.91     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | N     | 8701 | KEG  | W7-O29  | -4.74 | 1.70        | 1.91     |
| 4   | A     | 503  | KEG  | P1-O19  | -4.73 | 1.38        | 1.54     |
| 4   | N     | 8703 | KEG  | W7-O29  | -4.73 | 1.70        | 1.91     |
| 4   | A     | 501  | KEG  | P1-O19  | -4.72 | 1.38        | 1.54     |
| 4   | N     | 8702 | KEG  | P1-O19  | -4.72 | 1.38        | 1.54     |
| 4   | A     | 503  | KEG  | W2-O2   | -4.72 | 1.58        | 1.71     |
| 4   | M     | 8703 | KEG  | W7-O29  | -4.72 | 1.70        | 1.91     |
| 4   | N     | 8702 | KEG  | W7-O29  | -4.71 | 1.70        | 1.91     |
| 4   | N     | 8701 | KEG  | P1-O19  | -4.71 | 1.38        | 1.54     |
| 4   | M     | 8701 | KEG  | P1-O19  | -4.71 | 1.38        | 1.54     |
| 4   | M     | 8703 | KEG  | P1-O19  | -4.71 | 1.38        | 1.54     |
| 4   | N     | 8705 | KEG  | P1-O19  | -4.71 | 1.38        | 1.54     |
| 4   | M     | 8702 | KEG  | P1-O19  | -4.70 | 1.38        | 1.54     |
| 4   | N     | 8702 | KEG  | W2-O2   | -4.70 | 1.58        | 1.71     |
| 4   | A     | 502  | KEG  | W2-O2   | -4.70 | 1.58        | 1.71     |
| 4   | N     | 8704 | KEG  | P1-O19  | -4.70 | 1.38        | 1.54     |
| 4   | N     | 8704 | KEG  | W2-O2   | -4.69 | 1.58        | 1.71     |
| 4   | A     | 502  | KEG  | P1-O19  | -4.67 | 1.38        | 1.54     |
| 4   | N     | 8701 | KEG  | W2-O2   | -4.67 | 1.58        | 1.71     |
| 4   | M     | 8701 | KEG  | W2-O2   | -4.67 | 1.58        | 1.71     |
| 4   | M     | 8702 | KEG  | W2-O2   | -4.67 | 1.58        | 1.71     |
| 4   | N     | 8703 | KEG  | W2-O2   | -4.67 | 1.58        | 1.71     |
| 4   | N     | 8705 | KEG  | W2-O2   | -4.66 | 1.58        | 1.71     |
| 4   | A     | 501  | KEG  | W2-O2   | -4.66 | 1.58        | 1.71     |
| 4   | M     | 8703 | KEG  | W2-O2   | -4.64 | 1.58        | 1.71     |
| 4   | A     | 502  | KEG  | W1-O23  | -4.49 | 1.71        | 1.93     |
| 4   | A     | 503  | KEG  | W1-O23  | -4.48 | 1.71        | 1.93     |
| 4   | M     | 8701 | KEG  | W1-O23  | -4.47 | 1.71        | 1.93     |
| 4   | N     | 8701 | KEG  | W1-O23  | -4.47 | 1.71        | 1.93     |
| 4   | N     | 8704 | KEG  | W1-O23  | -4.47 | 1.71        | 1.93     |
| 4   | A     | 501  | KEG  | W1-O23  | -4.47 | 1.71        | 1.93     |
| 4   | M     | 8703 | KEG  | W1-O23  | -4.46 | 1.71        | 1.93     |
| 4   | A     | 502  | KEG  | W10-O18 | -4.46 | 2.19        | 2.43     |
| 4   | N     | 8702 | KEG  | W1-O23  | -4.46 | 1.71        | 1.93     |
| 4   | N     | 8705 | KEG  | W1-O23  | -4.46 | 1.71        | 1.93     |
| 4   | N     | 8703 | KEG  | W1-O23  | -4.45 | 1.71        | 1.93     |
| 4   | M     | 8702 | KEG  | W1-O23  | -4.45 | 1.71        | 1.93     |
| 4   | A     | 501  | KEG  | W10-O18 | -4.44 | 2.19        | 2.43     |
| 4   | M     | 8702 | KEG  | W10-O18 | -4.44 | 2.19        | 2.43     |
| 4   | M     | 8703 | KEG  | W10-O18 | -4.43 | 2.19        | 2.43     |
| 4   | A     | 503  | KEG  | W10-O18 | -4.43 | 2.19        | 2.43     |
| 4   | N     | 8703 | KEG  | W10-O18 | -4.43 | 2.19        | 2.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | N     | 8704 | KEG  | W10-O18 | -4.42 | 2.19        | 2.43     |
| 4   | M     | 8701 | KEG  | W10-O18 | -4.42 | 2.19        | 2.43     |
| 4   | N     | 8701 | KEG  | W10-O18 | -4.42 | 2.19        | 2.43     |
| 4   | N     | 8705 | KEG  | W10-O18 | -4.41 | 2.19        | 2.43     |
| 4   | N     | 8702 | KEG  | W10-O18 | -4.41 | 2.19        | 2.43     |
| 4   | N     | 8701 | KEG  | W2-O18  | -4.35 | 2.19        | 2.43     |
| 4   | M     | 8702 | KEG  | W2-O18  | -4.35 | 2.19        | 2.43     |
| 4   | N     | 8705 | KEG  | W2-O18  | -4.34 | 2.19        | 2.43     |
| 4   | M     | 8703 | KEG  | W2-O18  | -4.34 | 2.19        | 2.43     |
| 4   | N     | 8702 | KEG  | W2-O18  | -4.34 | 2.19        | 2.43     |
| 4   | A     | 502  | KEG  | W2-O18  | -4.33 | 2.19        | 2.43     |
| 4   | N     | 8703 | KEG  | W2-O18  | -4.33 | 2.19        | 2.43     |
| 4   | A     | 501  | KEG  | W2-O18  | -4.33 | 2.19        | 2.43     |
| 4   | A     | 503  | KEG  | W2-O18  | -4.32 | 2.19        | 2.43     |
| 4   | N     | 8704 | KEG  | W2-O18  | -4.32 | 2.19        | 2.43     |
| 4   | M     | 8701 | KEG  | W2-O18  | -4.31 | 2.19        | 2.43     |
| 4   | A     | 503  | KEG  | W11-O13 | -4.16 | 1.60        | 1.71     |
| 4   | A     | 501  | KEG  | W11-O13 | -4.16 | 1.60        | 1.71     |
| 4   | N     | 8705 | KEG  | W11-O13 | -4.16 | 1.60        | 1.71     |
| 4   | N     | 8704 | KEG  | W11-O13 | -4.15 | 1.60        | 1.71     |
| 4   | N     | 8703 | KEG  | W11-O13 | -4.15 | 1.60        | 1.71     |
| 4   | M     | 8703 | KEG  | W11-O13 | -4.15 | 1.60        | 1.71     |
| 4   | N     | 8701 | KEG  | W11-O13 | -4.15 | 1.60        | 1.71     |
| 4   | M     | 8701 | KEG  | W11-O13 | -4.14 | 1.60        | 1.71     |
| 4   | N     | 8702 | KEG  | W11-O13 | -4.14 | 1.60        | 1.71     |
| 4   | M     | 8702 | KEG  | W11-O13 | -4.13 | 1.60        | 1.71     |
| 4   | A     | 502  | KEG  | W11-O13 | -4.13 | 1.60        | 1.71     |
| 4   | A     | 502  | KEG  | W12-O14 | -4.04 | 1.60        | 1.71     |
| 4   | M     | 8702 | KEG  | W9-O42  | -4.03 | 1.73        | 1.91     |
| 4   | A     | 503  | KEG  | W9-O42  | -4.03 | 1.73        | 1.91     |
| 4   | N     | 8705 | KEG  | W9-O42  | -4.03 | 1.73        | 1.91     |
| 4   | N     | 8701 | KEG  | W9-O42  | -4.03 | 1.73        | 1.91     |
| 4   | M     | 8701 | KEG  | W9-O42  | -4.02 | 1.73        | 1.91     |
| 4   | N     | 8702 | KEG  | W9-O42  | -4.02 | 1.73        | 1.91     |
| 4   | A     | 501  | KEG  | W9-O42  | -4.02 | 1.73        | 1.91     |
| 4   | N     | 8704 | KEG  | W9-O42  | -4.01 | 1.73        | 1.91     |
| 4   | A     | 502  | KEG  | W9-O42  | -4.01 | 1.73        | 1.91     |
| 4   | N     | 8703 | KEG  | W9-O42  | -4.01 | 1.73        | 1.91     |
| 4   | A     | 501  | KEG  | W12-O14 | -4.01 | 1.60        | 1.71     |
| 4   | M     | 8701 | KEG  | W12-O14 | -4.01 | 1.60        | 1.71     |
| 4   | N     | 8702 | KEG  | W12-O14 | -4.00 | 1.60        | 1.71     |
| 4   | A     | 503  | KEG  | W12-O14 | -4.00 | 1.60        | 1.71     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | M     | 8702 | KEG  | W12-O14 | -4.00 | 1.60        | 1.71     |
| 4   | N     | 8705 | KEG  | W12-O14 | -3.99 | 1.60        | 1.71     |
| 4   | M     | 8703 | KEG  | W9-O42  | -3.99 | 1.74        | 1.91     |
| 4   | M     | 8703 | KEG  | W12-O14 | -3.99 | 1.60        | 1.71     |
| 4   | N     | 8704 | KEG  | W12-O14 | -3.97 | 1.60        | 1.71     |
| 4   | N     | 8701 | KEG  | W12-O14 | -3.96 | 1.60        | 1.71     |
| 4   | N     | 8703 | KEG  | W12-O14 | -3.96 | 1.60        | 1.71     |
| 4   | A     | 502  | KEG  | W10-O36 | -3.86 | 1.74        | 1.93     |
| 4   | N     | 8702 | KEG  | W10-O36 | -3.85 | 1.74        | 1.93     |
| 4   | M     | 8701 | KEG  | W10-O36 | -3.85 | 1.74        | 1.93     |
| 4   | N     | 8704 | KEG  | W10-O36 | -3.85 | 1.74        | 1.93     |
| 4   | M     | 8703 | KEG  | W10-O36 | -3.84 | 1.74        | 1.93     |
| 4   | A     | 501  | KEG  | W10-O36 | -3.84 | 1.74        | 1.93     |
| 4   | N     | 8701 | KEG  | W10-O36 | -3.84 | 1.74        | 1.93     |
| 4   | M     | 8702 | KEG  | W10-O36 | -3.84 | 1.74        | 1.93     |
| 4   | N     | 8705 | KEG  | W10-O36 | -3.84 | 1.74        | 1.93     |
| 4   | N     | 8703 | KEG  | W10-O36 | -3.84 | 1.74        | 1.93     |
| 4   | A     | 503  | KEG  | W10-O36 | -3.83 | 1.74        | 1.93     |
| 4   | M     | 8703 | KEG  | W1-O17  | -3.83 | 2.22        | 2.43     |
| 4   | A     | 502  | KEG  | W1-O17  | -3.82 | 2.22        | 2.43     |
| 4   | N     | 8705 | KEG  | W1-O17  | -3.82 | 2.22        | 2.43     |
| 4   | M     | 8702 | KEG  | W1-O17  | -3.82 | 2.22        | 2.43     |
| 4   | N     | 8703 | KEG  | W1-O17  | -3.82 | 2.22        | 2.43     |
| 4   | M     | 8701 | KEG  | W1-O17  | -3.82 | 2.22        | 2.43     |
| 4   | A     | 501  | KEG  | W1-O17  | -3.82 | 2.22        | 2.43     |
| 4   | N     | 8701 | KEG  | W1-O17  | -3.81 | 2.22        | 2.43     |
| 4   | A     | 503  | KEG  | W1-O17  | -3.80 | 2.22        | 2.43     |
| 4   | N     | 8704 | KEG  | W1-O17  | -3.80 | 2.22        | 2.43     |
| 4   | N     | 8702 | KEG  | W1-O17  | -3.79 | 2.22        | 2.43     |
| 4   | A     | 502  | KEG  | W8-O10  | -3.68 | 1.61        | 1.71     |
| 4   | N     | 8704 | KEG  | W8-O10  | -3.65 | 1.61        | 1.71     |
| 4   | N     | 8701 | KEG  | W8-O10  | -3.65 | 1.61        | 1.71     |
| 4   | M     | 8701 | KEG  | W8-O10  | -3.64 | 1.61        | 1.71     |
| 4   | N     | 8702 | KEG  | W8-O10  | -3.63 | 1.61        | 1.71     |
| 4   | A     | 503  | KEG  | W8-O10  | -3.62 | 1.61        | 1.71     |
| 4   | N     | 8705 | KEG  | W8-O10  | -3.61 | 1.61        | 1.71     |
| 4   | M     | 8702 | KEG  | W8-O10  | -3.61 | 1.61        | 1.71     |
| 4   | N     | 8703 | KEG  | W8-O10  | -3.60 | 1.61        | 1.71     |
| 4   | A     | 501  | KEG  | W8-O10  | -3.60 | 1.61        | 1.71     |
| 4   | M     | 8703 | KEG  | W8-O10  | -3.60 | 1.61        | 1.71     |
| 4   | A     | 501  | KEG  | W6-O24  | -3.41 | 1.76        | 1.93     |
| 4   | M     | 8701 | KEG  | W6-O24  | -3.41 | 1.76        | 1.93     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | A     | 502  | KEG  | W6-O24 | -3.39 | 1.77        | 1.93     |
| 4   | N     | 8704 | KEG  | W6-O24 | -3.38 | 1.77        | 1.93     |
| 4   | M     | 8702 | KEG  | W6-O24 | -3.38 | 1.77        | 1.93     |
| 4   | A     | 503  | KEG  | W6-O24 | -3.38 | 1.77        | 1.93     |
| 4   | M     | 8703 | KEG  | W6-O24 | -3.38 | 1.77        | 1.93     |
| 4   | A     | 502  | KEG  | W3-O21 | 3.37  | 2.61        | 2.43     |
| 4   | N     | 8703 | KEG  | W6-O24 | -3.37 | 1.77        | 1.93     |
| 4   | N     | 8705 | KEG  | W6-O24 | -3.37 | 1.77        | 1.93     |
| 4   | N     | 8701 | KEG  | W6-O24 | -3.36 | 1.77        | 1.93     |
| 4   | N     | 8702 | KEG  | W6-O24 | -3.36 | 1.77        | 1.93     |
| 4   | N     | 8705 | KEG  | W3-O21 | 3.35  | 2.61        | 2.43     |
| 4   | A     | 503  | KEG  | W3-O21 | 3.35  | 2.61        | 2.43     |
| 4   | M     | 8701 | KEG  | W3-O21 | 3.35  | 2.61        | 2.43     |
| 4   | N     | 8704 | KEG  | W3-O21 | 3.35  | 2.61        | 2.43     |
| 4   | N     | 8701 | KEG  | W3-O21 | 3.35  | 2.61        | 2.43     |
| 4   | A     | 501  | KEG  | W3-O21 | 3.35  | 2.61        | 2.43     |
| 4   | N     | 8703 | KEG  | W3-O21 | 3.34  | 2.61        | 2.43     |
| 4   | M     | 8703 | KEG  | W3-O21 | 3.33  | 2.61        | 2.43     |
| 4   | M     | 8702 | KEG  | W3-O21 | 3.33  | 2.61        | 2.43     |
| 4   | N     | 8702 | KEG  | W3-O21 | 3.33  | 2.61        | 2.43     |
| 4   | N     | 8703 | KEG  | W2-O24 | -3.15 | 1.78        | 1.93     |
| 4   | N     | 8701 | KEG  | W2-O24 | -3.14 | 1.78        | 1.93     |
| 4   | N     | 8702 | KEG  | W2-O24 | -3.13 | 1.78        | 1.93     |
| 4   | N     | 8704 | KEG  | W2-O24 | -3.13 | 1.78        | 1.93     |
| 4   | N     | 8701 | KEG  | W9-O11 | -3.13 | 1.62        | 1.71     |
| 4   | N     | 8704 | KEG  | W9-O11 | -3.12 | 1.62        | 1.71     |
| 4   | N     | 8705 | KEG  | W2-O24 | -3.12 | 1.78        | 1.93     |
| 4   | A     | 503  | KEG  | W2-O24 | -3.12 | 1.78        | 1.93     |
| 4   | M     | 8703 | KEG  | W2-O24 | -3.12 | 1.78        | 1.93     |
| 4   | M     | 8701 | KEG  | W2-O24 | -3.12 | 1.78        | 1.93     |
| 4   | M     | 8703 | KEG  | W9-O11 | -3.12 | 1.63        | 1.71     |
| 4   | A     | 501  | KEG  | W2-O24 | -3.11 | 1.78        | 1.93     |
| 4   | A     | 502  | KEG  | W2-O24 | -3.11 | 1.78        | 1.93     |
| 4   | A     | 501  | KEG  | W9-O11 | -3.11 | 1.63        | 1.71     |
| 4   | M     | 8702 | KEG  | W2-O24 | -3.11 | 1.78        | 1.93     |
| 4   | M     | 8702 | KEG  | W9-O11 | -3.10 | 1.63        | 1.71     |
| 4   | A     | 502  | KEG  | W9-O11 | -3.09 | 1.63        | 1.71     |
| 4   | N     | 8703 | KEG  | W9-O11 | -3.09 | 1.63        | 1.71     |
| 4   | A     | 503  | KEG  | W9-O11 | -3.09 | 1.63        | 1.71     |
| 4   | N     | 8705 | KEG  | W9-O11 | -3.08 | 1.63        | 1.71     |
| 4   | M     | 8701 | KEG  | W9-O11 | -3.07 | 1.63        | 1.71     |
| 4   | N     | 8702 | KEG  | W9-O11 | -3.05 | 1.63        | 1.71     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | N     | 8703 | KEG  | W3-O25  | -3.03 | 1.78        | 1.91     |
| 4   | N     | 8705 | KEG  | W3-O25  | -3.03 | 1.78        | 1.91     |
| 4   | M     | 8703 | KEG  | W3-O25  | -3.02 | 1.78        | 1.91     |
| 4   | M     | 8701 | KEG  | W3-O25  | -3.02 | 1.78        | 1.91     |
| 4   | N     | 8704 | KEG  | W3-O25  | -3.02 | 1.78        | 1.91     |
| 4   | N     | 8701 | KEG  | W3-O25  | -3.02 | 1.78        | 1.91     |
| 4   | A     | 501  | KEG  | W3-O25  | -3.02 | 1.78        | 1.91     |
| 4   | A     | 503  | KEG  | W3-O25  | -3.02 | 1.78        | 1.91     |
| 4   | M     | 8702 | KEG  | W3-O25  | -3.02 | 1.78        | 1.91     |
| 4   | N     | 8702 | KEG  | W3-O25  | -3.01 | 1.78        | 1.91     |
| 4   | A     | 502  | KEG  | W3-O25  | -3.01 | 1.78        | 1.91     |
| 4   | N     | 8705 | KEG  | W10-O12 | -2.93 | 1.63        | 1.71     |
| 4   | N     | 8702 | KEG  | W10-O12 | -2.93 | 1.63        | 1.71     |
| 4   | N     | 8702 | KEG  | W8-O44  | -2.93 | 1.79        | 1.93     |
| 4   | N     | 8703 | KEG  | W10-O12 | -2.92 | 1.63        | 1.71     |
| 4   | N     | 8701 | KEG  | W10-O12 | -2.92 | 1.63        | 1.71     |
| 4   | N     | 8703 | KEG  | W8-O44  | -2.92 | 1.79        | 1.93     |
| 4   | N     | 8704 | KEG  | W8-O44  | -2.92 | 1.79        | 1.93     |
| 4   | M     | 8701 | KEG  | W8-O44  | -2.91 | 1.79        | 1.93     |
| 4   | A     | 502  | KEG  | W8-O44  | -2.91 | 1.79        | 1.93     |
| 4   | M     | 8703 | KEG  | W8-O44  | -2.91 | 1.79        | 1.93     |
| 4   | A     | 501  | KEG  | W8-O44  | -2.91 | 1.79        | 1.93     |
| 4   | M     | 8701 | KEG  | W10-O12 | -2.90 | 1.63        | 1.71     |
| 4   | N     | 8701 | KEG  | W8-O44  | -2.89 | 1.79        | 1.93     |
| 4   | A     | 503  | KEG  | W8-O44  | -2.89 | 1.79        | 1.93     |
| 4   | M     | 8702 | KEG  | W8-O44  | -2.89 | 1.79        | 1.93     |
| 4   | M     | 8703 | KEG  | W10-O12 | -2.89 | 1.63        | 1.71     |
| 4   | N     | 8704 | KEG  | W10-O12 | -2.89 | 1.63        | 1.71     |
| 4   | A     | 501  | KEG  | W10-O12 | -2.88 | 1.63        | 1.71     |
| 4   | M     | 8702 | KEG  | W10-O12 | -2.88 | 1.63        | 1.71     |
| 4   | N     | 8705 | KEG  | W8-O44  | -2.87 | 1.79        | 1.93     |
| 4   | A     | 503  | KEG  | W10-O12 | -2.86 | 1.63        | 1.71     |
| 4   | M     | 8703 | KEG  | W6-O8   | -2.85 | 1.63        | 1.71     |
| 4   | A     | 502  | KEG  | W10-O12 | -2.85 | 1.63        | 1.71     |
| 4   | N     | 8704 | KEG  | W6-O8   | -2.84 | 1.63        | 1.71     |
| 4   | N     | 8702 | KEG  | W6-O8   | -2.84 | 1.63        | 1.71     |
| 4   | N     | 8703 | KEG  | W6-O8   | -2.83 | 1.63        | 1.71     |
| 4   | M     | 8701 | KEG  | W6-O8   | -2.83 | 1.63        | 1.71     |
| 4   | A     | 502  | KEG  | W6-O8   | -2.83 | 1.63        | 1.71     |
| 4   | N     | 8705 | KEG  | W6-O8   | -2.82 | 1.63        | 1.71     |
| 4   | A     | 501  | KEG  | W6-O8   | -2.82 | 1.63        | 1.71     |
| 4   | M     | 8702 | KEG  | W6-O8   | -2.82 | 1.63        | 1.71     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | N     | 8701 | KEG  | W6-O8  | -2.82 | 1.63        | 1.71     |
| 4   | A     | 503  | KEG  | W6-O8  | -2.79 | 1.63        | 1.71     |
| 4   | A     | 501  | KEG  | W3-O37 | 2.79  | 2.07        | 1.93     |
| 4   | N     | 8704 | KEG  | W3-O37 | 2.78  | 2.07        | 1.93     |
| 4   | N     | 8703 | KEG  | W3-O37 | 2.78  | 2.07        | 1.93     |
| 4   | N     | 8705 | KEG  | W3-O37 | 2.78  | 2.07        | 1.93     |
| 4   | M     | 8701 | KEG  | W3-O37 | 2.77  | 2.07        | 1.93     |
| 4   | A     | 502  | KEG  | W3-O37 | 2.77  | 2.07        | 1.93     |
| 4   | M     | 8703 | KEG  | W3-O37 | 2.77  | 2.07        | 1.93     |
| 4   | A     | 503  | KEG  | W3-O37 | 2.76  | 2.07        | 1.93     |
| 4   | N     | 8701 | KEG  | W3-O37 | 2.76  | 2.07        | 1.93     |
| 4   | M     | 8702 | KEG  | W3-O37 | 2.76  | 2.07        | 1.93     |
| 4   | N     | 8702 | KEG  | W3-O37 | 2.75  | 2.07        | 1.93     |
| 4   | N     | 8704 | KEG  | W5-O7  | -2.75 | 1.64        | 1.71     |
| 4   | A     | 502  | KEG  | W5-O7  | -2.73 | 1.64        | 1.71     |
| 4   | M     | 8703 | KEG  | W5-O7  | -2.72 | 1.64        | 1.71     |
| 4   | M     | 8701 | KEG  | W5-O7  | -2.71 | 1.64        | 1.71     |
| 4   | A     | 503  | KEG  | W5-O7  | -2.71 | 1.64        | 1.71     |
| 4   | M     | 8702 | KEG  | W5-O7  | -2.71 | 1.64        | 1.71     |
| 4   | N     | 8703 | KEG  | W5-O7  | -2.70 | 1.64        | 1.71     |
| 4   | N     | 8705 | KEG  | W5-O7  | -2.70 | 1.64        | 1.71     |
| 4   | N     | 8701 | KEG  | W5-O7  | -2.68 | 1.64        | 1.71     |
| 4   | N     | 8702 | KEG  | W5-O7  | -2.68 | 1.64        | 1.71     |
| 4   | A     | 501  | KEG  | W5-O7  | -2.67 | 1.64        | 1.71     |
| 4   | N     | 8704 | KEG  | P1-O21 | 2.59  | 1.63        | 1.54     |
| 4   | N     | 8703 | KEG  | P1-O21 | 2.58  | 1.63        | 1.54     |
| 4   | M     | 8702 | KEG  | P1-O21 | 2.57  | 1.63        | 1.54     |
| 4   | N     | 8702 | KEG  | P1-O21 | 2.57  | 1.63        | 1.54     |
| 4   | A     | 503  | KEG  | W1-O1  | -2.57 | 1.64        | 1.71     |
| 4   | N     | 8701 | KEG  | P1-O21 | 2.56  | 1.63        | 1.54     |
| 4   | A     | 503  | KEG  | P1-O21 | 2.56  | 1.63        | 1.54     |
| 4   | M     | 8703 | KEG  | P1-O21 | 2.56  | 1.63        | 1.54     |
| 4   | N     | 8701 | KEG  | W1-O1  | -2.56 | 1.64        | 1.71     |
| 4   | N     | 8705 | KEG  | P1-O21 | 2.55  | 1.63        | 1.54     |
| 4   | A     | 501  | KEG  | P1-O21 | 2.55  | 1.63        | 1.54     |
| 4   | N     | 8703 | KEG  | W1-O1  | -2.55 | 1.64        | 1.71     |
| 4   | N     | 8705 | KEG  | W1-O1  | -2.54 | 1.64        | 1.71     |
| 4   | M     | 8701 | KEG  | P1-O21 | 2.54  | 1.63        | 1.54     |
| 4   | A     | 502  | KEG  | P1-O21 | 2.54  | 1.63        | 1.54     |
| 4   | M     | 8701 | KEG  | W1-O1  | -2.53 | 1.64        | 1.71     |
| 4   | N     | 8702 | KEG  | W1-O1  | -2.52 | 1.64        | 1.71     |
| 4   | A     | 502  | KEG  | W1-O1  | -2.52 | 1.64        | 1.71     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | M     | 8703 | KEG  | W11-O40 | -2.52 | 1.80        | 1.91     |
| 4   | A     | 502  | KEG  | W11-O40 | -2.52 | 1.80        | 1.91     |
| 4   | M     | 8702 | KEG  | W1-O1   | -2.52 | 1.64        | 1.71     |
| 4   | M     | 8702 | KEG  | W11-O40 | -2.52 | 1.80        | 1.91     |
| 4   | N     | 8703 | KEG  | W11-O40 | -2.51 | 1.80        | 1.91     |
| 4   | A     | 501  | KEG  | W1-O1   | -2.51 | 1.64        | 1.71     |
| 4   | M     | 8701 | KEG  | W11-O40 | -2.51 | 1.80        | 1.91     |
| 4   | M     | 8703 | KEG  | W1-O1   | -2.51 | 1.64        | 1.71     |
| 4   | A     | 503  | KEG  | W11-O40 | -2.51 | 1.80        | 1.91     |
| 4   | N     | 8701 | KEG  | W11-O40 | -2.51 | 1.80        | 1.91     |
| 4   | A     | 501  | KEG  | W11-O40 | -2.51 | 1.80        | 1.91     |
| 4   | N     | 8704 | KEG  | W11-O40 | -2.51 | 1.80        | 1.91     |
| 4   | N     | 8702 | KEG  | W11-O40 | -2.51 | 1.80        | 1.91     |
| 4   | N     | 8704 | KEG  | W1-O1   | -2.50 | 1.64        | 1.71     |
| 4   | N     | 8705 | KEG  | W11-O40 | -2.50 | 1.80        | 1.91     |
| 4   | A     | 502  | KEG  | W5-O32  | 2.44  | 2.01        | 1.91     |
| 4   | A     | 503  | KEG  | W5-O32  | 2.44  | 2.01        | 1.91     |
| 4   | M     | 8703 | KEG  | W5-O32  | 2.43  | 2.01        | 1.91     |
| 4   | N     | 8703 | KEG  | W5-O32  | 2.43  | 2.01        | 1.91     |
| 4   | M     | 8701 | KEG  | W5-O32  | 2.43  | 2.01        | 1.91     |
| 4   | M     | 8702 | KEG  | W5-O32  | 2.43  | 2.01        | 1.91     |
| 4   | N     | 8701 | KEG  | W5-O32  | 2.42  | 2.01        | 1.91     |
| 4   | N     | 8702 | KEG  | W5-O32  | 2.42  | 2.01        | 1.91     |
| 4   | A     | 501  | KEG  | W5-O32  | 2.41  | 2.01        | 1.91     |
| 4   | N     | 8704 | KEG  | W5-O32  | 2.41  | 2.01        | 1.91     |
| 4   | N     | 8705 | KEG  | W5-O32  | 2.40  | 2.01        | 1.91     |
| 4   | M     | 8702 | KEG  | W4-O6   | -2.39 | 1.64        | 1.71     |
| 4   | A     | 501  | KEG  | W4-O6   | -2.37 | 1.65        | 1.71     |
| 4   | N     | 8702 | KEG  | W4-O6   | -2.37 | 1.65        | 1.71     |
| 4   | N     | 8702 | KEG  | W4-O21  | 2.36  | 2.55        | 2.43     |
| 4   | N     | 8705 | KEG  | W4-O6   | -2.36 | 1.65        | 1.71     |
| 4   | A     | 501  | KEG  | W4-O21  | 2.35  | 2.55        | 2.43     |
| 4   | A     | 502  | KEG  | W4-O6   | -2.35 | 1.65        | 1.71     |
| 4   | N     | 8701 | KEG  | W4-O6   | -2.35 | 1.65        | 1.71     |
| 4   | M     | 8702 | KEG  | W4-O21  | 2.35  | 2.55        | 2.43     |
| 4   | M     | 8703 | KEG  | W4-O21  | 2.34  | 2.55        | 2.43     |
| 4   | A     | 503  | KEG  | W4-O6   | -2.34 | 1.65        | 1.71     |
| 4   | N     | 8703 | KEG  | W4-O21  | 2.34  | 2.55        | 2.43     |
| 4   | N     | 8704 | KEG  | W4-O6   | -2.34 | 1.65        | 1.71     |
| 4   | A     | 502  | KEG  | W4-O21  | 2.34  | 2.55        | 2.43     |
| 4   | M     | 8701 | KEG  | W4-O21  | 2.34  | 2.55        | 2.43     |
| 4   | N     | 8701 | KEG  | W4-O21  | 2.34  | 2.55        | 2.43     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | M     | 8701 | KEG  | W4-O6  | -2.33 | 1.65        | 1.71     |
| 4   | N     | 8703 | KEG  | W4-O6  | -2.33 | 1.65        | 1.71     |
| 4   | A     | 503  | KEG  | W4-O21 | 2.33  | 2.55        | 2.43     |
| 4   | N     | 8704 | KEG  | W4-O21 | 2.33  | 2.55        | 2.43     |
| 4   | M     | 8701 | KEG  | W6-O32 | 2.32  | 2.01        | 1.91     |
| 4   | N     | 8705 | KEG  | W4-O21 | 2.32  | 2.55        | 2.43     |
| 4   | A     | 501  | KEG  | W6-O32 | 2.31  | 2.01        | 1.91     |
| 4   | N     | 8704 | KEG  | W6-O32 | 2.31  | 2.01        | 1.91     |
| 4   | M     | 8703 | KEG  | W4-O6  | -2.31 | 1.65        | 1.71     |
| 4   | A     | 502  | KEG  | W6-O32 | 2.31  | 2.01        | 1.91     |
| 4   | N     | 8703 | KEG  | W6-O32 | 2.30  | 2.01        | 1.91     |
| 4   | N     | 8702 | KEG  | W1-O25 | -2.30 | 1.81        | 1.91     |
| 4   | M     | 8702 | KEG  | W1-O25 | -2.29 | 1.81        | 1.91     |
| 4   | N     | 8705 | KEG  | W6-O32 | 2.29  | 2.01        | 1.91     |
| 4   | M     | 8702 | KEG  | W6-O32 | 2.29  | 2.01        | 1.91     |
| 4   | M     | 8701 | KEG  | W1-O25 | -2.29 | 1.81        | 1.91     |
| 4   | M     | 8703 | KEG  | W1-O25 | -2.29 | 1.81        | 1.91     |
| 4   | M     | 8703 | KEG  | W6-O32 | 2.28  | 2.01        | 1.91     |
| 4   | N     | 8705 | KEG  | W1-O25 | -2.28 | 1.81        | 1.91     |
| 4   | N     | 8701 | KEG  | W7-O33 | -2.28 | 1.81        | 1.91     |
| 4   | N     | 8702 | KEG  | W6-O32 | 2.28  | 2.01        | 1.91     |
| 4   | N     | 8704 | KEG  | W1-O25 | -2.28 | 1.81        | 1.91     |
| 4   | N     | 8703 | KEG  | W1-O25 | -2.28 | 1.81        | 1.91     |
| 4   | N     | 8702 | KEG  | W7-O33 | -2.27 | 1.81        | 1.91     |
| 4   | N     | 8701 | KEG  | W1-O25 | -2.27 | 1.81        | 1.91     |
| 4   | A     | 503  | KEG  | W6-O32 | 2.27  | 2.01        | 1.91     |
| 4   | N     | 8701 | KEG  | W6-O32 | 2.27  | 2.00        | 1.91     |
| 4   | A     | 502  | KEG  | W1-O25 | -2.27 | 1.81        | 1.91     |
| 4   | N     | 8703 | KEG  | W7-O33 | -2.27 | 1.81        | 1.91     |
| 4   | A     | 502  | KEG  | W4-O26 | -2.27 | 1.81        | 1.91     |
| 4   | N     | 8704 | KEG  | W7-O33 | -2.27 | 1.81        | 1.91     |
| 4   | M     | 8703 | KEG  | W7-O33 | -2.26 | 1.81        | 1.91     |
| 4   | N     | 8705 | KEG  | W7-O33 | -2.26 | 1.81        | 1.91     |
| 4   | N     | 8701 | KEG  | W4-O26 | -2.26 | 1.81        | 1.91     |
| 4   | M     | 8701 | KEG  | W4-O26 | -2.26 | 1.81        | 1.91     |
| 4   | M     | 8702 | KEG  | W4-O26 | -2.26 | 1.81        | 1.91     |
| 4   | A     | 503  | KEG  | W7-O33 | -2.25 | 1.81        | 1.91     |
| 4   | M     | 8703 | KEG  | W4-O26 | -2.25 | 1.81        | 1.91     |
| 4   | N     | 8705 | KEG  | W4-O26 | -2.25 | 1.81        | 1.91     |
| 4   | A     | 501  | KEG  | W1-O25 | -2.25 | 1.81        | 1.91     |
| 4   | A     | 502  | KEG  | W7-O33 | -2.25 | 1.81        | 1.91     |
| 4   | A     | 501  | KEG  | W7-O33 | -2.24 | 1.81        | 1.91     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | N     | 8704 | KEG  | W4-O26  | -2.24 | 1.81        | 1.91     |
| 4   | A     | 503  | KEG  | W1-O25  | -2.24 | 1.81        | 1.91     |
| 4   | M     | 8701 | KEG  | W7-O33  | -2.24 | 1.81        | 1.91     |
| 4   | N     | 8703 | KEG  | W4-O26  | -2.24 | 1.81        | 1.91     |
| 4   | A     | 501  | KEG  | W4-O26  | -2.24 | 1.81        | 1.91     |
| 4   | N     | 8702 | KEG  | W4-O26  | -2.24 | 1.81        | 1.91     |
| 4   | A     | 503  | KEG  | W4-O26  | -2.23 | 1.81        | 1.91     |
| 4   | A     | 502  | KEG  | W2-O26  | -2.23 | 1.81        | 1.91     |
| 4   | A     | 503  | KEG  | W2-O26  | -2.22 | 1.81        | 1.91     |
| 4   | N     | 8704 | KEG  | W2-O26  | -2.22 | 1.81        | 1.91     |
| 4   | M     | 8702 | KEG  | W7-O33  | -2.22 | 1.81        | 1.91     |
| 4   | A     | 501  | KEG  | W2-O26  | -2.22 | 1.81        | 1.91     |
| 4   | M     | 8702 | KEG  | W2-O26  | -2.21 | 1.81        | 1.91     |
| 4   | N     | 8701 | KEG  | W2-O26  | -2.21 | 1.81        | 1.91     |
| 4   | N     | 8702 | KEG  | W2-O26  | -2.21 | 1.81        | 1.91     |
| 4   | N     | 8705 | KEG  | W2-O26  | -2.21 | 1.81        | 1.91     |
| 4   | M     | 8701 | KEG  | W2-O26  | -2.20 | 1.81        | 1.91     |
| 4   | M     | 8703 | KEG  | W2-O26  | -2.20 | 1.81        | 1.91     |
| 4   | M     | 8702 | KEG  | W11-O44 | -2.19 | 1.82        | 1.93     |
| 4   | N     | 8704 | KEG  | W8-O41  | -2.19 | 1.82        | 1.93     |
| 4   | N     | 8702 | KEG  | W8-O41  | -2.18 | 1.82        | 1.93     |
| 4   | N     | 8703 | KEG  | W2-O26  | -2.18 | 1.81        | 1.91     |
| 4   | M     | 8701 | KEG  | W8-O41  | -2.17 | 1.82        | 1.93     |
| 4   | N     | 8705 | KEG  | W8-O41  | -2.17 | 1.83        | 1.93     |
| 4   | N     | 8702 | KEG  | W11-O44 | -2.17 | 1.83        | 1.93     |
| 4   | A     | 501  | KEG  | W8-O41  | -2.17 | 1.83        | 1.93     |
| 4   | N     | 8705 | KEG  | W11-O44 | -2.17 | 1.83        | 1.93     |
| 4   | A     | 503  | KEG  | W11-O44 | -2.17 | 1.83        | 1.93     |
| 4   | M     | 8703 | KEG  | W11-O44 | -2.17 | 1.83        | 1.93     |
| 4   | M     | 8702 | KEG  | W8-O41  | -2.16 | 1.83        | 1.93     |
| 4   | N     | 8703 | KEG  | W8-O41  | -2.16 | 1.83        | 1.93     |
| 4   | N     | 8701 | KEG  | W11-O44 | -2.16 | 1.83        | 1.93     |
| 4   | M     | 8703 | KEG  | W8-O41  | -2.16 | 1.83        | 1.93     |
| 4   | A     | 503  | KEG  | W8-O41  | -2.16 | 1.83        | 1.93     |
| 4   | N     | 8701 | KEG  | W8-O41  | -2.15 | 1.83        | 1.93     |
| 4   | N     | 8703 | KEG  | W11-O44 | -2.15 | 1.83        | 1.93     |
| 4   | N     | 8704 | KEG  | W11-O44 | -2.15 | 1.83        | 1.93     |
| 4   | A     | 502  | KEG  | W11-O44 | -2.15 | 1.83        | 1.93     |
| 4   | A     | 501  | KEG  | W11-O44 | -2.15 | 1.83        | 1.93     |
| 4   | A     | 502  | KEG  | W8-O41  | -2.15 | 1.83        | 1.93     |
| 4   | M     | 8701 | KEG  | W11-O44 | -2.15 | 1.83        | 1.93     |
| 4   | M     | 8703 | KEG  | W3-O31  | 2.01  | 2.03        | 1.93     |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4   | M     | 8701 | KEG  | O19-P1-O18 | -2.23 | 104.65      | 108.92   |
| 4   | N     | 8705 | KEG  | O19-P1-O18 | -2.23 | 104.65      | 108.92   |
| 4   | N     | 8702 | KEG  | O19-P1-O18 | -2.22 | 104.68      | 108.92   |
| 4   | A     | 502  | KEG  | O19-P1-O18 | -2.20 | 104.71      | 108.92   |
| 4   | M     | 8703 | KEG  | O19-P1-O18 | -2.19 | 104.74      | 108.92   |
| 4   | N     | 8704 | KEG  | O19-P1-O18 | -2.18 | 104.74      | 108.92   |
| 4   | A     | 501  | KEG  | O19-P1-O18 | -2.18 | 104.74      | 108.92   |
| 4   | M     | 8702 | KEG  | O19-P1-O18 | -2.18 | 104.75      | 108.92   |
| 4   | N     | 8703 | KEG  | O19-P1-O18 | -2.18 | 104.75      | 108.92   |
| 4   | N     | 8701 | KEG  | O19-P1-O18 | -2.17 | 104.77      | 108.92   |
| 4   | A     | 503  | KEG  | O19-P1-O18 | -2.16 | 104.79      | 108.92   |
| 4   | M     | 8701 | KEG  | O21-P1-O18 | 2.12  | 112.97      | 108.92   |
| 4   | M     | 8703 | KEG  | O21-P1-O18 | 2.10  | 112.95      | 108.92   |
| 4   | N     | 8705 | KEG  | O21-P1-O18 | 2.10  | 112.94      | 108.92   |
| 4   | N     | 8704 | KEG  | O21-P1-O18 | 2.10  | 112.93      | 108.92   |
| 4   | A     | 501  | KEG  | O21-P1-O18 | 2.09  | 112.93      | 108.92   |
| 4   | N     | 8701 | KEG  | O21-P1-O18 | 2.09  | 112.92      | 108.92   |
| 4   | N     | 8703 | KEG  | O21-P1-O18 | 2.08  | 112.91      | 108.92   |
| 4   | A     | 503  | KEG  | O21-P1-O18 | 2.08  | 112.90      | 108.92   |
| 4   | M     | 8702 | KEG  | O21-P1-O18 | 2.08  | 112.90      | 108.92   |
| 4   | A     | 502  | KEG  | O21-P1-O18 | 2.07  | 112.89      | 108.92   |
| 4   | N     | 8702 | KEG  | O21-P1-O18 | 2.07  | 112.89      | 108.92   |

There are no chirality outliers.

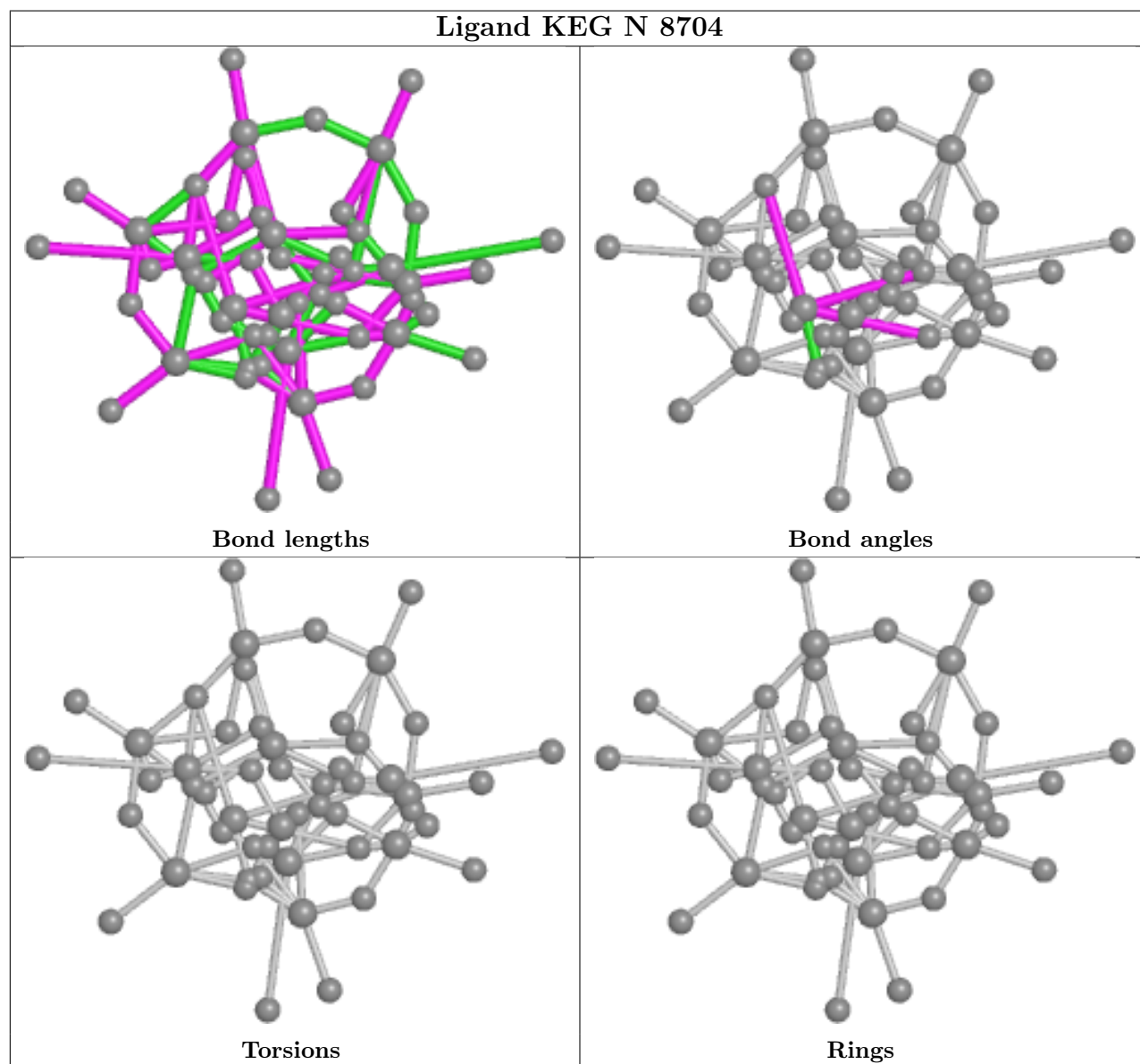
There are no torsion outliers.

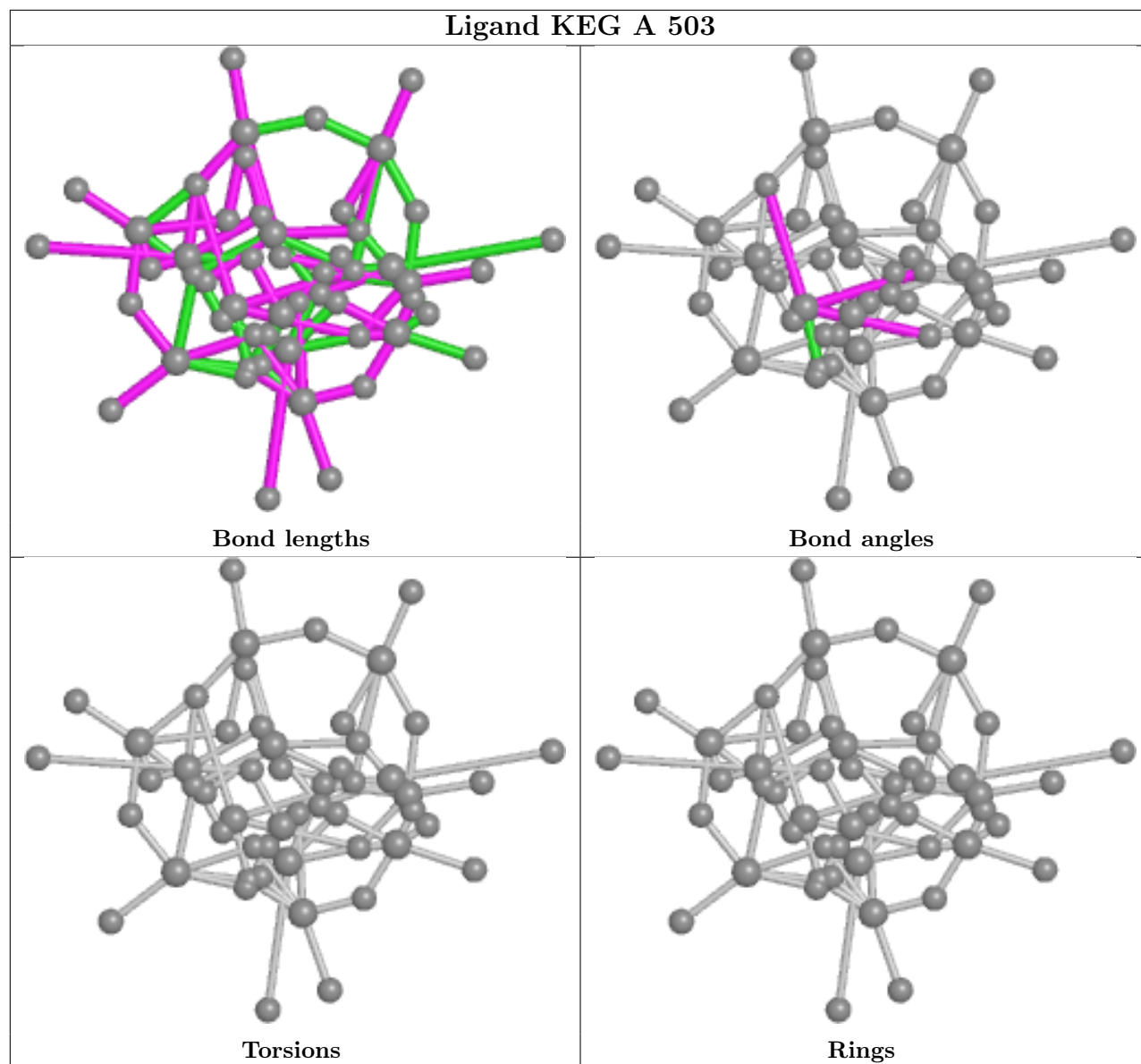
There are no ring outliers.

11 monomers are involved in 101 short contacts:

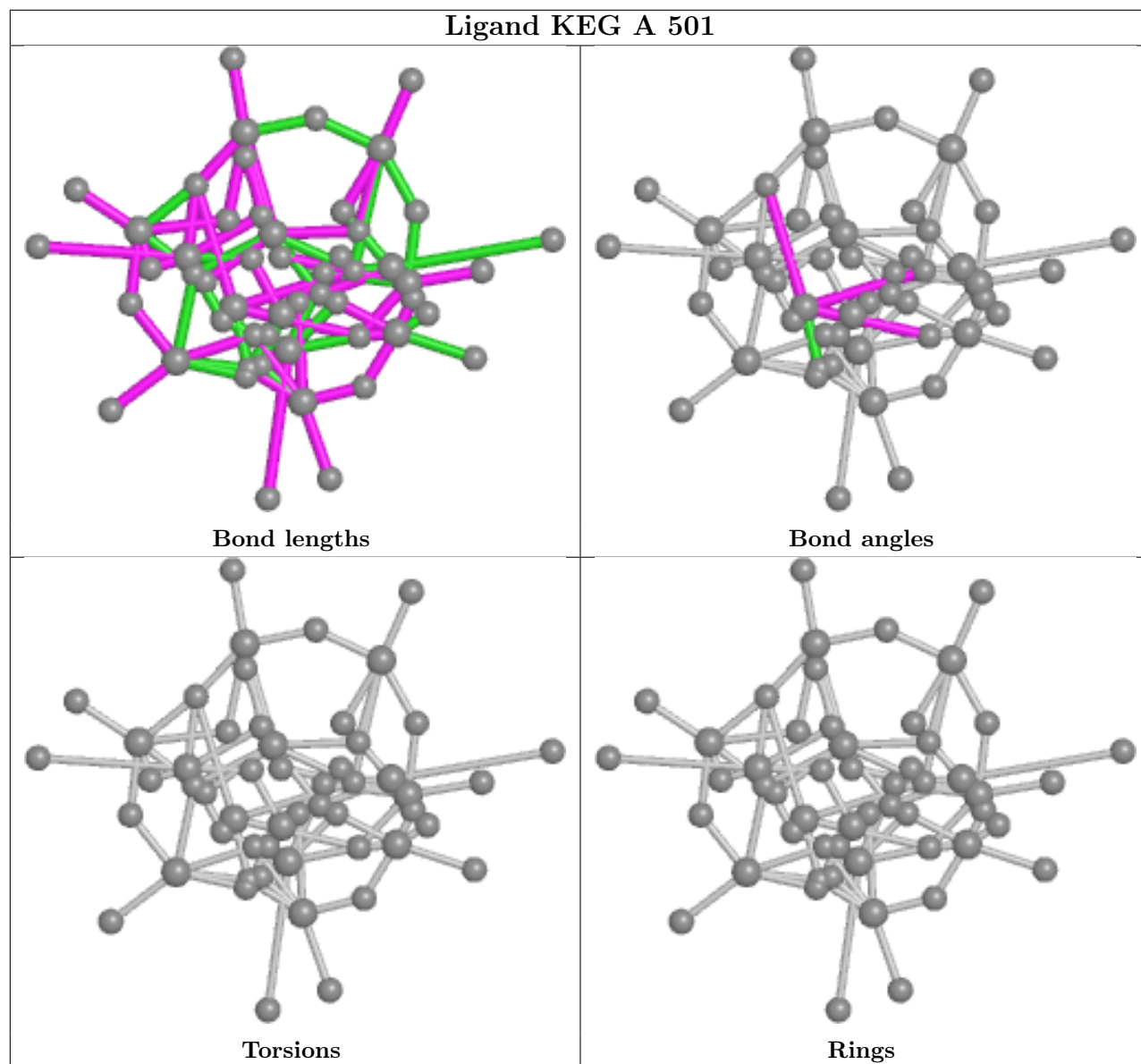
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | N     | 8704 | KEG  | 6       | 0            |
| 4   | A     | 503  | KEG  | 16      | 0            |
| 4   | A     | 501  | KEG  | 24      | 0            |
| 4   | N     | 8703 | KEG  | 6       | 0            |
| 4   | A     | 502  | KEG  | 13      | 0            |
| 4   | M     | 8703 | KEG  | 6       | 0            |
| 4   | N     | 8702 | KEG  | 6       | 0            |
| 4   | M     | 8702 | KEG  | 6       | 0            |
| 4   | M     | 8701 | KEG  | 6       | 0            |
| 4   | N     | 8705 | KEG  | 6       | 0            |
| 4   | N     | 8701 | KEG  | 6       | 0            |

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



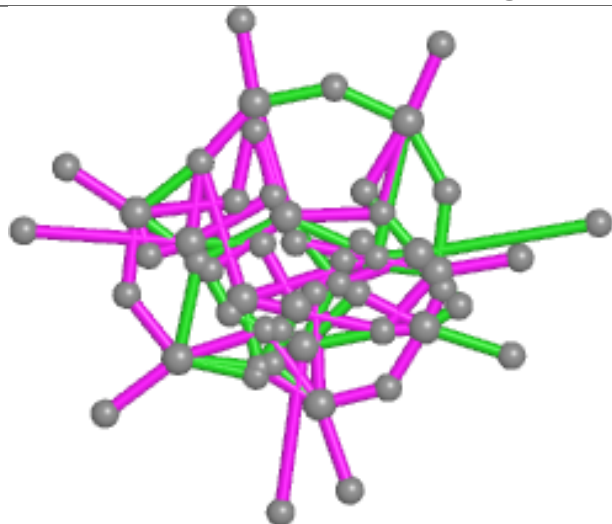




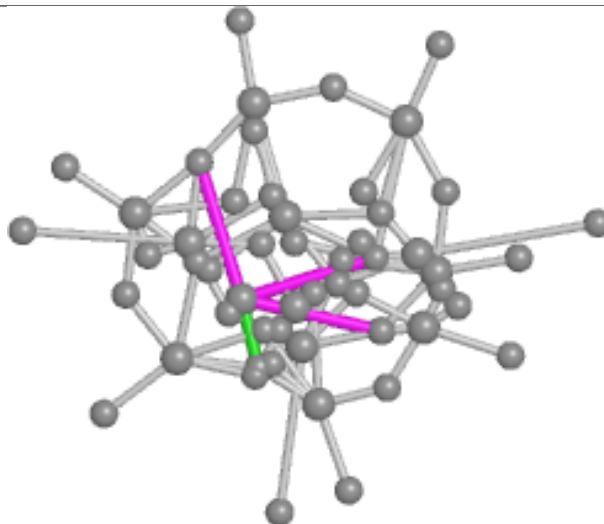




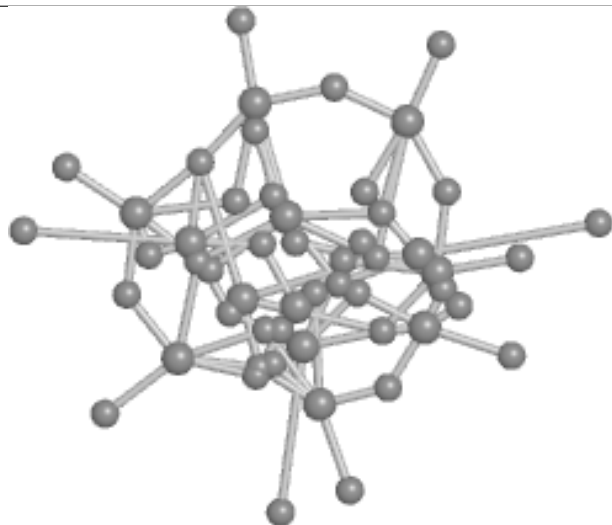
## Ligand KEG N 8703



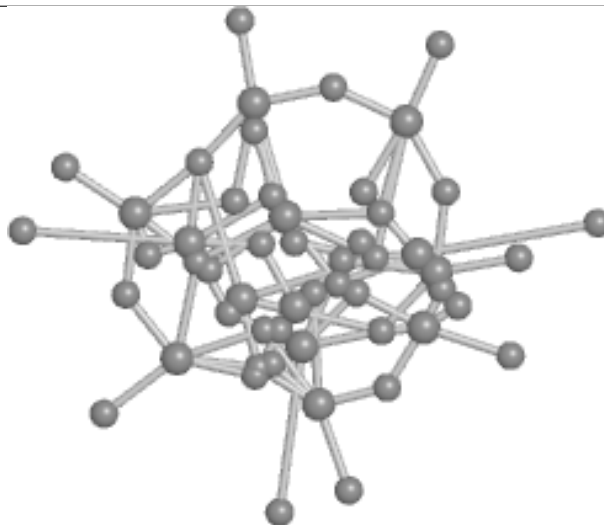
Bond lengths



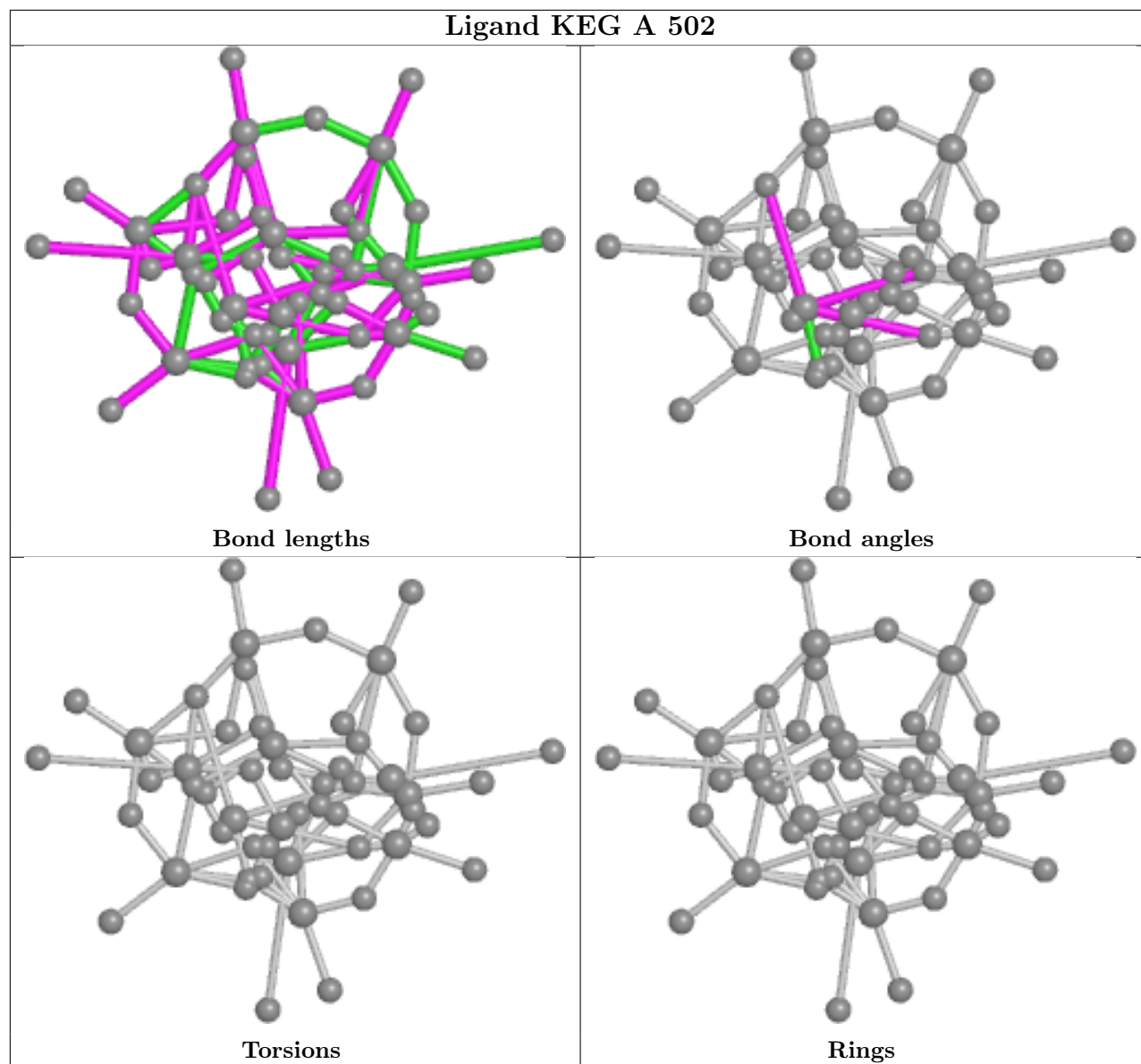
Bond angles



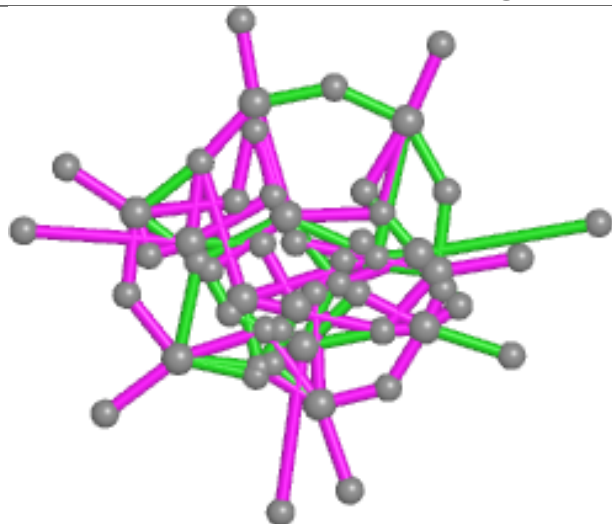
Torsions



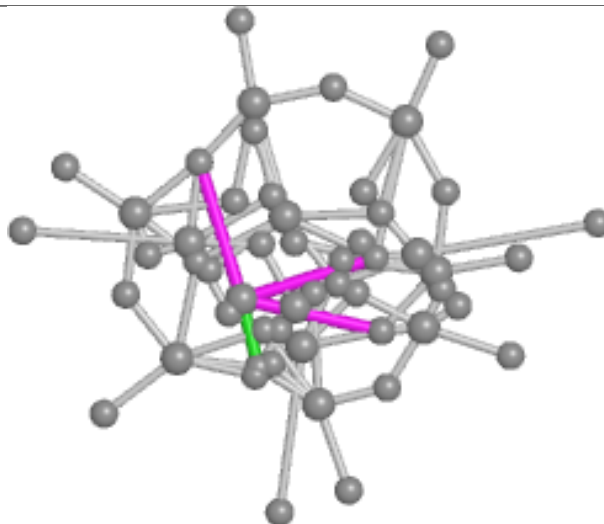
Rings



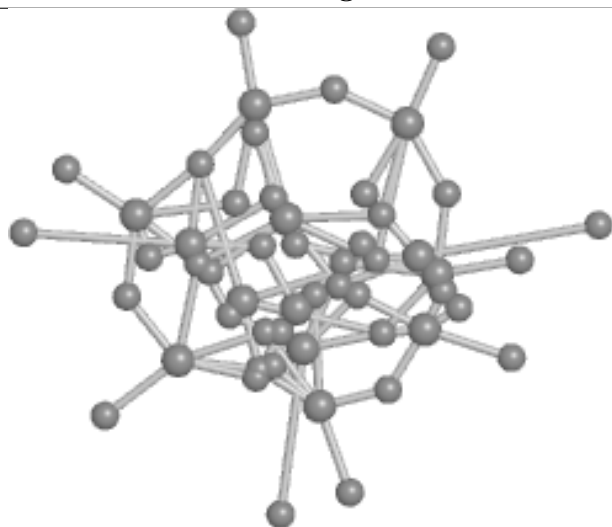
## Ligand KEG M 8703



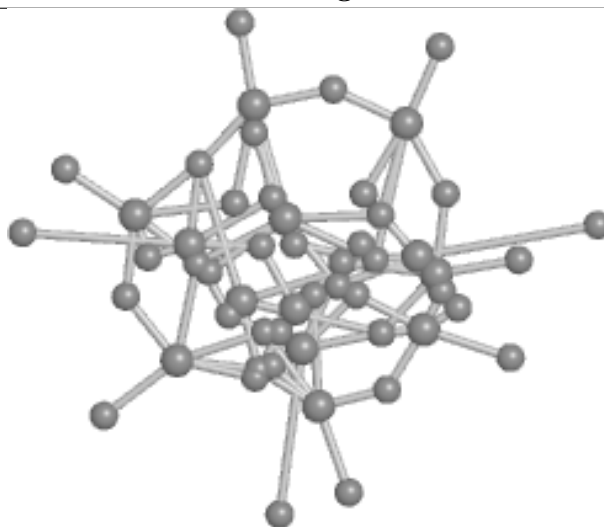
Bond lengths



Bond angles

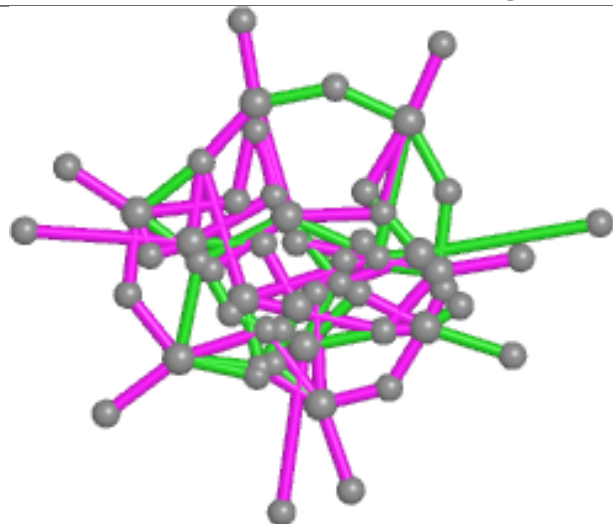


Torsions

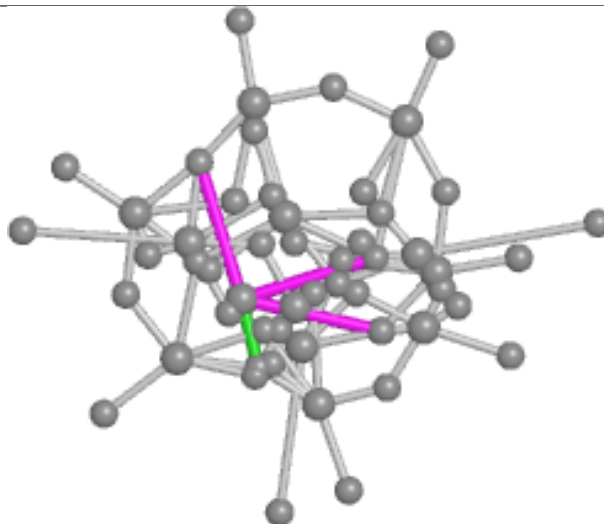


Rings

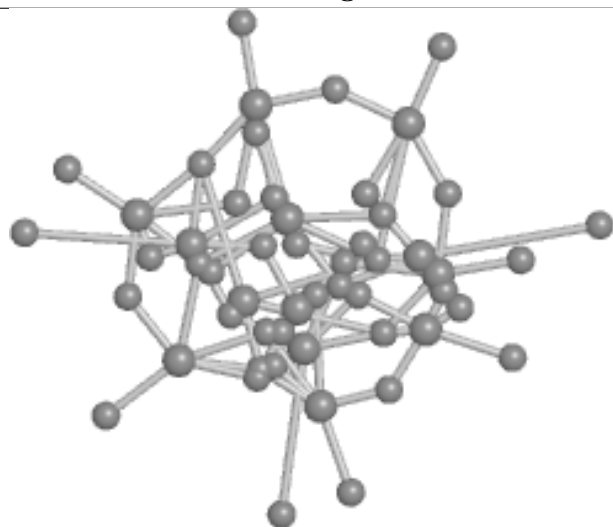
## Ligand KEG N 8702



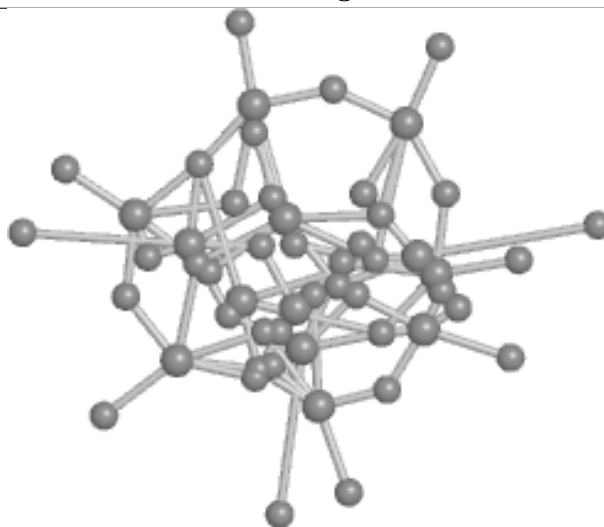
Bond lengths



Bond angles

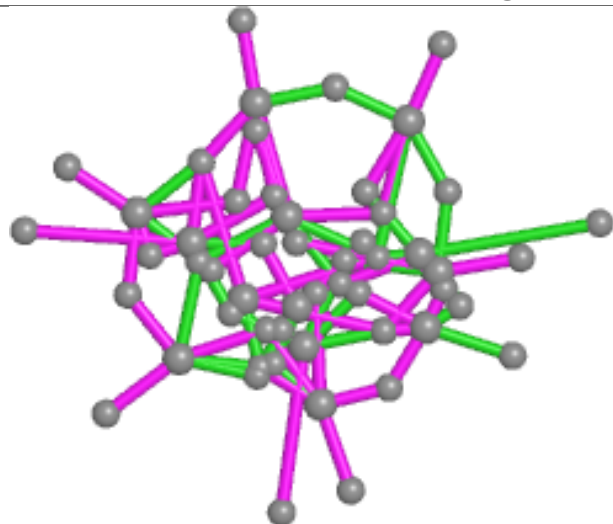


Torsions

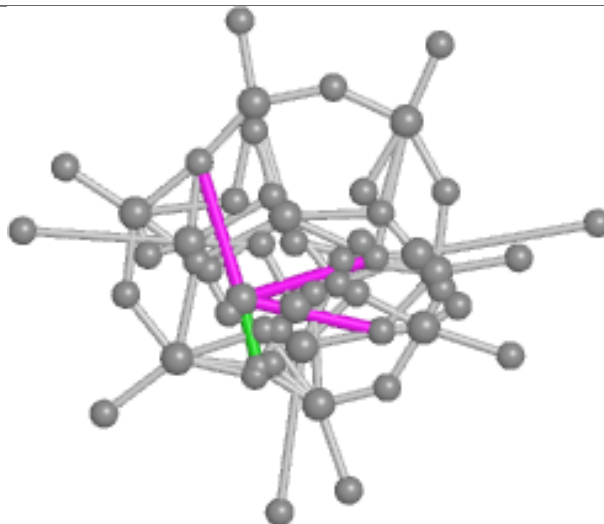


Rings

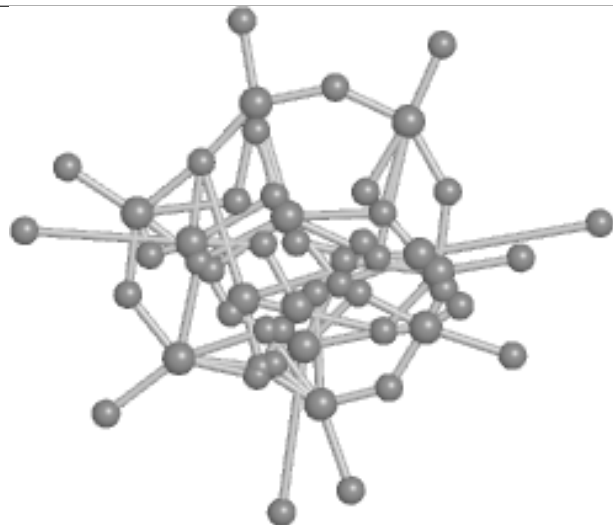
## Ligand KEG M 8702



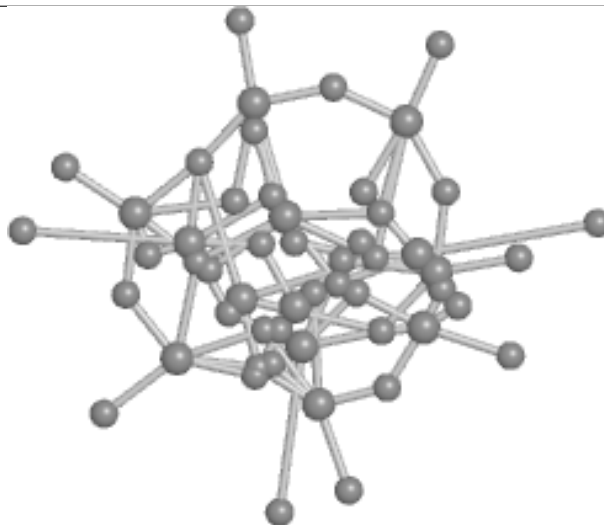
Bond lengths



Bond angles

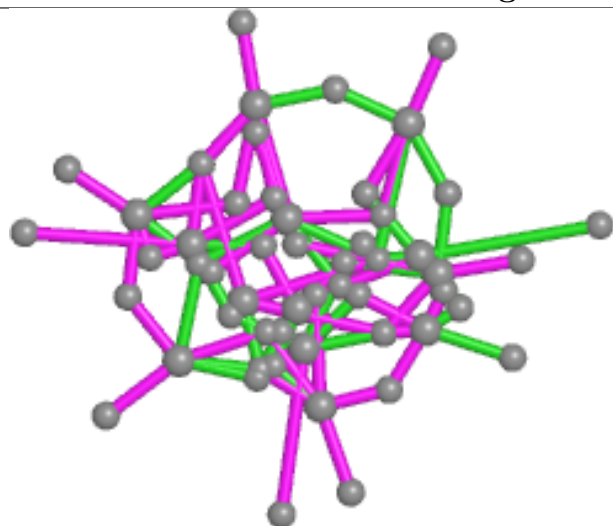


Torsions

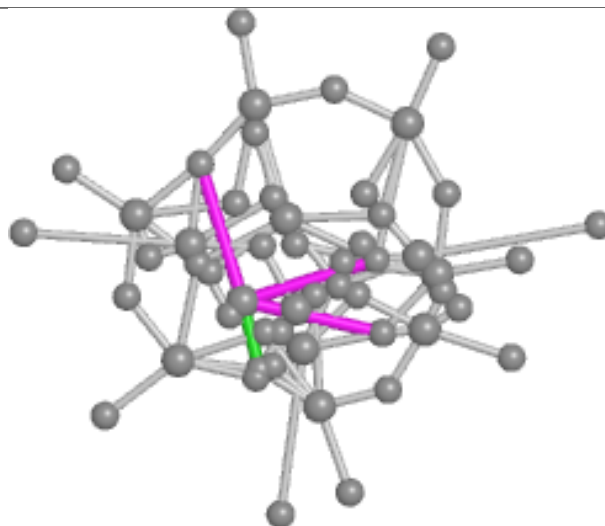


Rings

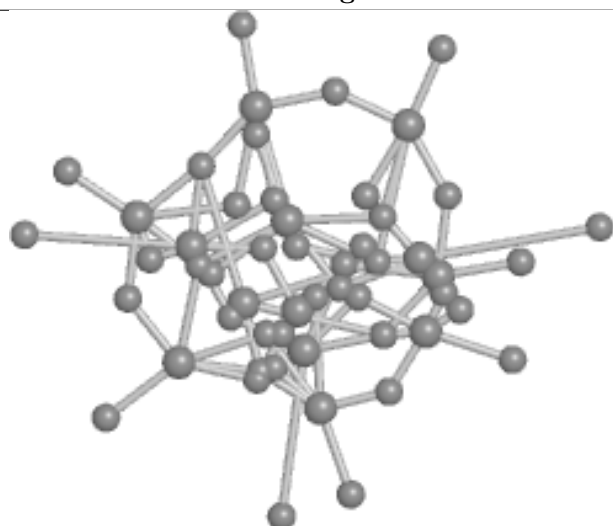
## Ligand KEG M 8701



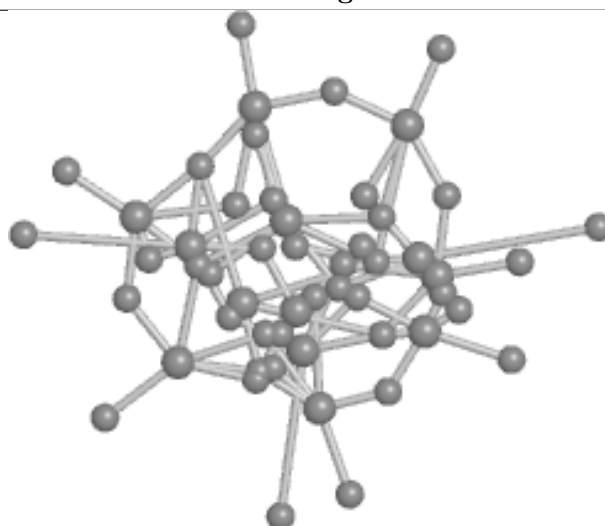
Bond lengths



Bond angles

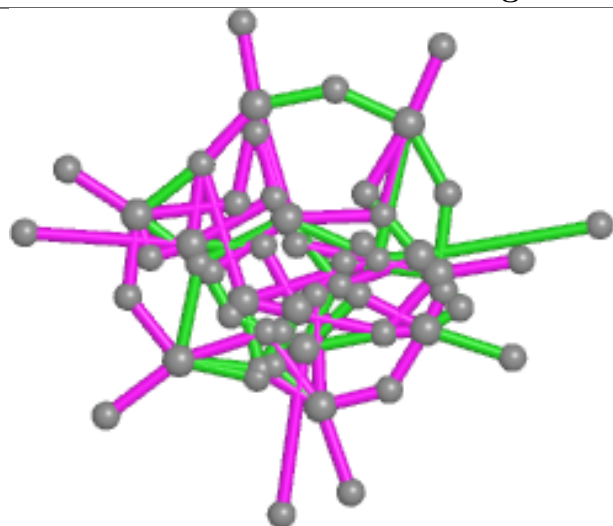


Torsions

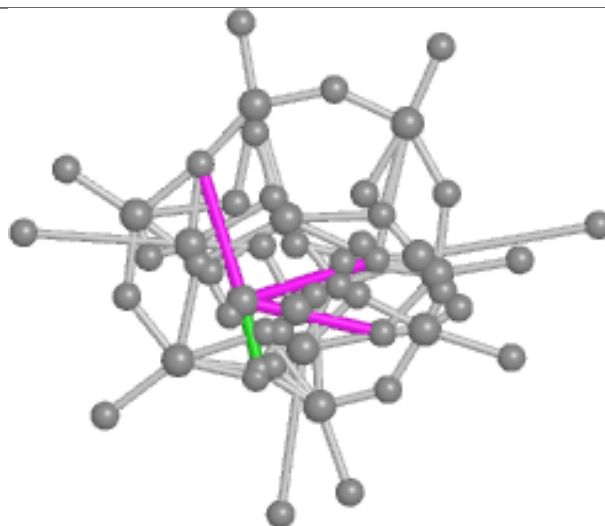


Rings

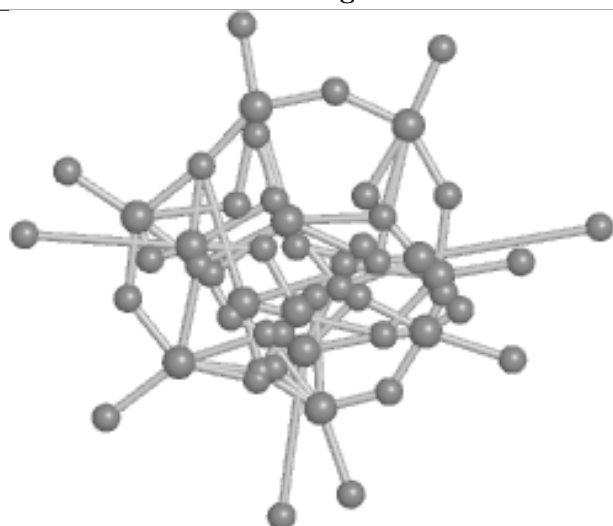
## Ligand KEG N 8705



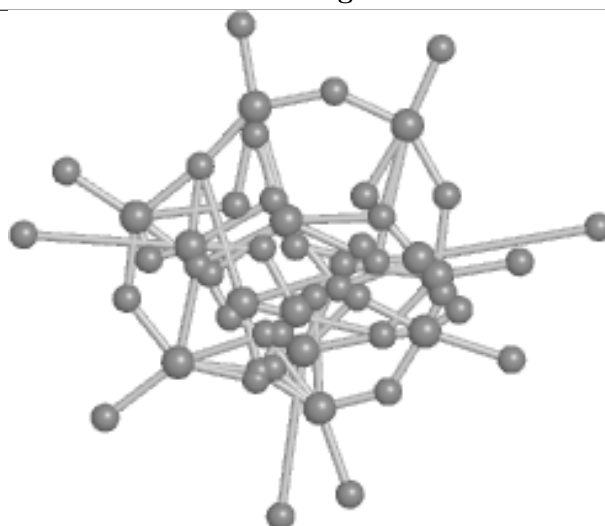
Bond lengths



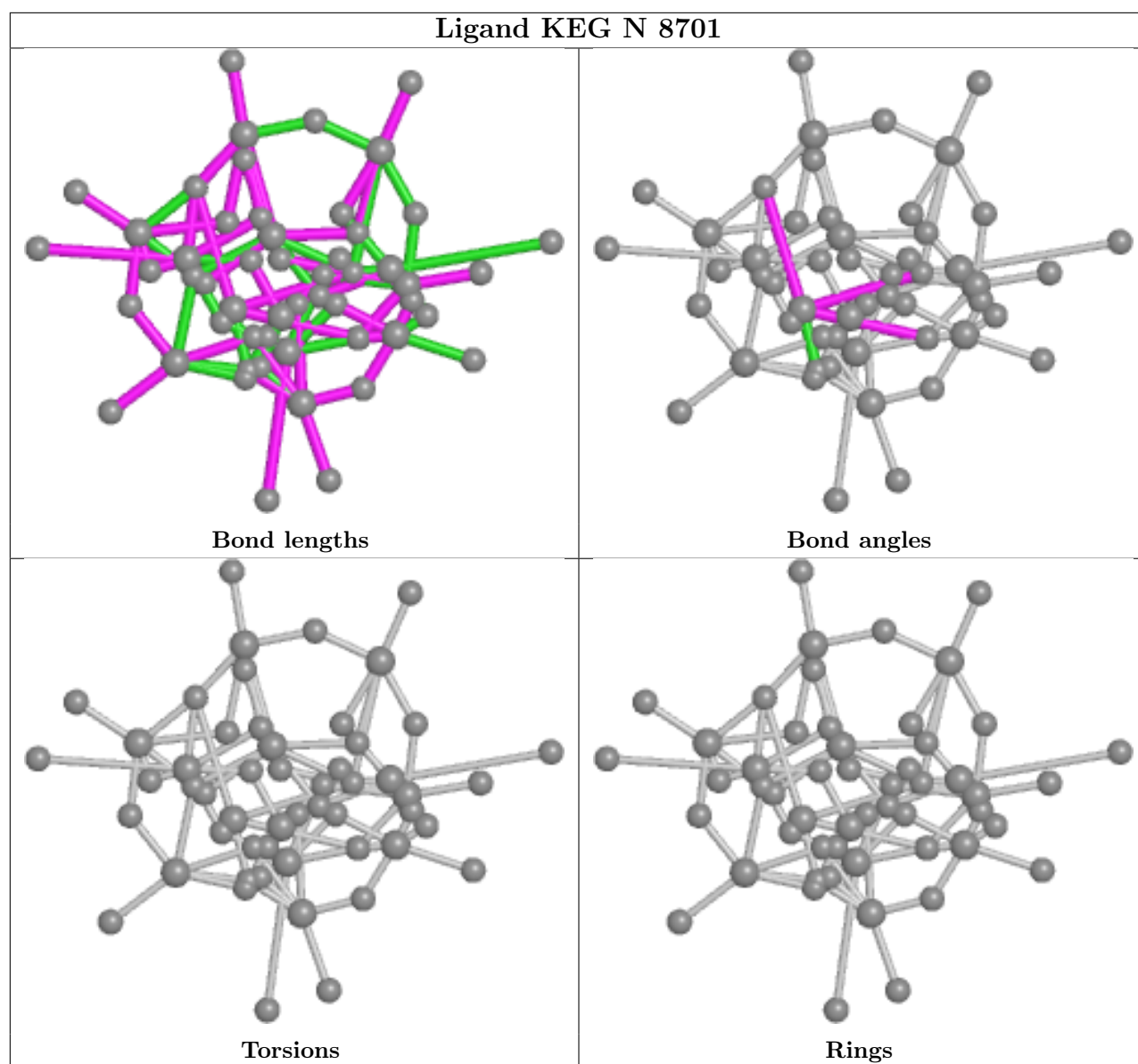
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | N     | 126              |
| 3   | M     | 126              |
| 2   | B     | 27               |
| 2   | D     | 27               |



All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | N     | 5289:UNK  | C      | 6033:UNK  | N      | 143.88       |
| 1     | M     | 5289:UNK  | C      | 6033:UNK  | N      | 142.81       |
| 1     | N     | 5148:UNK  | C      | 5197:UNK  | N      | 119.38       |
| 1     | M     | 5148:UNK  | C      | 5197:UNK  | N      | 119.33       |
| 1     | N     | 492:UNK   | C      | 2104:UNK  | N      | 118.52       |
| 1     | M     | 492:UNK   | C      | 2104:UNK  | N      | 116.29       |
| 1     | N     | 2121:UNK  | C      | 2503:UNK  | N      | 113.46       |
| 1     | M     | 2121:UNK  | C      | 2503:UNK  | N      | 110.84       |
| 1     | M     | 4017:UNK  | C      | 4063:UNK  | N      | 96.53        |
| 1     | N     | 4017:UNK  | C      | 4063:UNK  | N      | 96.53        |
| 1     | N     | 3052:UNK  | C      | 3180:UNK  | N      | 87.26        |
| 1     | M     | 3052:UNK  | C      | 3180:UNK  | N      | 87.14        |
| 1     | M     | 2992:UNK  | C      | 3011:UNK  | N      | 66.88        |
| 1     | N     | 2992:UNK  | C      | 3011:UNK  | N      | 66.88        |
| 1     | N     | 7362:UNK  | C      | 8092:UNK  | N      | 66.56        |
| 1     | M     | 7362:UNK  | C      | 8092:UNK  | N      | 66.31        |
| 1     | M     | 6744:UNK  | C      | 6808:UNK  | N      | 65.65        |
| 1     | N     | 6744:UNK  | C      | 6808:UNK  | N      | 65.65        |
| 1     | M     | 2846:UNK  | C      | 2857:UNK  | N      | 58.81        |
| 1     | N     | 2846:UNK  | C      | 2857:UNK  | N      | 58.81        |
| 1     | M     | 2958:UNK  | C      | 2971:UNK  | N      | 58.36        |
| 1     | N     | 2958:UNK  | C      | 2971:UNK  | N      | 58.36        |
| 1     | M     | 2927:UNK  | C      | 2938:UNK  | N      | 56.61        |
| 1     | M     | 221:UNK   | C      | 232:UNK   | N      | 56.04        |
| 1     | N     | 221:UNK   | C      | 232:UNK   | N      | 56.04        |
| 1     | N     | 2927:UNK  | C      | 2938:UNK  | N      | 55.65        |
| 1     | M     | 3200:UNK  | C      | 4002:UNK  | N      | 55.11        |
| 1     | N     | 3200:UNK  | C      | 4002:UNK  | N      | 54.88        |
| 1     | M     | 7079:UNK  | C      | 7103:UNK  | N      | 52.41        |
| 1     | N     | 7079:UNK  | C      | 7103:UNK  | N      | 52.41        |
| 1     | M     | 6081:UNK  | C      | 6092:UNK  | N      | 49.92        |
| 1     | N     | 6081:UNK  | C      | 6092:UNK  | N      | 49.92        |
| 1     | M     | 6871:UNK  | C      | 6877:UNK  | N      | 43.24        |
| 1     | N     | 6871:UNK  | C      | 6877:UNK  | N      | 43.24        |
| 1     | M     | 8498:UNK  | C      | 8539:UNK  | N      | 41.00        |
| 1     | N     | 8498:UNK  | C      | 8539:UNK  | N      | 41.00        |
| 1     | M     | 6502:UNK  | C      | 6514:UNK  | N      | 39.49        |
| 1     | N     | 6502:UNK  | C      | 6514:UNK  | N      | 39.49        |
| 1     | M     | 4105:UNK  | C      | 4110:UNK  | N      | 38.22        |
| 1     | N     | 4105:UNK  | C      | 4110:UNK  | N      | 38.21        |
| 1     | M     | 2681:UNK  | C      | 2800:UNK  | N      | 38.17        |
| 1     | M     | 4618:UNK  | C      | 4629:UNK  | N      | 38.07        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | N     | 4618:UNK  | C      | 4629:UNK  | N      | 38.07        |
| 1     | M     | 4734:UNK  | C      | 4746:UNK  | N      | 37.66        |
| 1     | N     | 4734:UNK  | C      | 4746:UNK  | N      | 37.66        |
| 1     | M     | 2523:UNK  | C      | 2537:UNK  | N      | 36.92        |
| 1     | N     | 2523:UNK  | C      | 2537:UNK  | N      | 36.92        |
| 1     | N     | 8253:UNK  | C      | 8256:UNK  | N      | 36.58        |
| 1     | M     | 4688:UNK  | C      | 4690:UNK  | N      | 36.49        |
| 1     | N     | 4688:UNK  | C      | 4690:UNK  | N      | 36.49        |
| 1     | N     | 2681:UNK  | C      | 2800:UNK  | N      | 36.35        |
| 1     | M     | 8253:UNK  | C      | 8256:UNK  | N      | 36.29        |
| 1     | M     | 2895:UNK  | C      | 2906:UNK  | N      | 36.08        |
| 1     | N     | 2895:UNK  | C      | 2906:UNK  | N      | 36.08        |
| 1     | M     | 471:UNK   | C      | 482:UNK   | N      | 35.36        |
| 1     | N     | 471:UNK   | C      | 482:UNK   | N      | 35.36        |
| 1     | M     | 8126:UNK  | C      | 8133:UNK  | N      | 35.02        |
| 1     | N     | 8126:UNK  | C      | 8133:UNK  | N      | 35.02        |
| 1     | M     | 6114:UNK  | C      | 6123:UNK  | N      | 34.38        |
| 1     | N     | 6114:UNK  | C      | 6123:UNK  | N      | 34.38        |
| 1     | M     | 4353:UNK  | C      | 4366:UNK  | N      | 34.34        |
| 1     | N     | 4353:UNK  | C      | 4366:UNK  | N      | 34.34        |
| 1     | M     | 6826:UNK  | C      | 6830:UNK  | N      | 34.23        |
| 1     | N     | 6826:UNK  | C      | 6830:UNK  | N      | 34.23        |
| 1     | M     | 6680:UNK  | C      | 6692:UNK  | N      | 33.69        |
| 1     | N     | 6680:UNK  | C      | 6692:UNK  | N      | 33.69        |
| 1     | M     | 411:UNK   | C      | 425:UNK   | N      | 33.36        |
| 1     | N     | 411:UNK   | C      | 425:UNK   | N      | 33.36        |
| 1     | M     | 6053:UNK  | C      | 6066:UNK  | N      | 32.68        |
| 1     | N     | 6053:UNK  | C      | 6066:UNK  | N      | 32.68        |
| 1     | M     | 4567:UNK  | C      | 4578:UNK  | N      | 31.33        |
| 1     | N     | 4567:UNK  | C      | 4578:UNK  | N      | 31.33        |
| 1     | M     | 4895:UNK  | C      | 4905:UNK  | N      | 30.94        |
| 1     | N     | 4895:UNK  | C      | 4905:UNK  | N      | 30.94        |
| 1     | M     | 4709:UNK  | C      | 4720:UNK  | N      | 30.88        |
| 1     | N     | 4709:UNK  | C      | 4720:UNK  | N      | 30.88        |
| 1     | M     | 4217:UNK  | C      | 4230:UNK  | N      | 30.33        |
| 1     | N     | 4217:UNK  | C      | 4230:UNK  | N      | 30.33        |
| 1     | M     | 6647:UNK  | C      | 6659:UNK  | N      | 29.73        |
| 1     | N     | 6647:UNK  | C      | 6659:UNK  | N      | 29.73        |
| 1     | M     | 4273:UNK  | C      | 4286:UNK  | N      | 29.70        |
| 1     | N     | 4273:UNK  | C      | 4286:UNK  | N      | 29.70        |
| 1     | M     | 4187:UNK  | C      | 4199:UNK  | N      | 29.38        |
| 1     | N     | 4187:UNK  | C      | 4199:UNK  | N      | 29.38        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 4443:UNK  | C      | 4454:UNK  | N      | 29.37        |
| 1     | M     | 4763:UNK  | C      | 4780:UNK  | N      | 29.37        |
| 1     | N     | 4443:UNK  | C      | 4454:UNK  | N      | 29.37        |
| 1     | N     | 4763:UNK  | C      | 4780:UNK  | N      | 29.37        |
| 1     | M     | 5238:UNK  | C      | 5251:UNK  | N      | 28.59        |
| 1     | N     | 5238:UNK  | C      | 5251:UNK  | N      | 28.59        |
| 1     | M     | 4244:UNK  | C      | 4255:UNK  | N      | 28.49        |
| 1     | N     | 4244:UNK  | C      | 4255:UNK  | N      | 28.49        |
| 1     | M     | 7222:UNK  | C      | 7342:UNK  | N      | 28.20        |
| 1     | N     | 7222:UNK  | C      | 7342:UNK  | N      | 28.20        |
| 1     | M     | 4472:UNK  | C      | 4484:UNK  | N      | 28.19        |
| 1     | N     | 4472:UNK  | C      | 4484:UNK  | N      | 28.19        |
| 1     | M     | 8299:UNK  | C      | 8311:UNK  | N      | 28.06        |
| 1     | N     | 8299:UNK  | C      | 8311:UNK  | N      | 28.06        |
| 1     | M     | 8226:UNK  | C      | 8234:UNK  | N      | 28.03        |
| 1     | N     | 8226:UNK  | C      | 8234:UNK  | N      | 28.03        |
| 1     | M     | 4076:UNK  | C      | 4089:UNK  | N      | 27.97        |
| 1     | N     | 4076:UNK  | C      | 4089:UNK  | N      | 27.97        |
| 1     | M     | 6468:UNK  | C      | 6480:UNK  | N      | 27.60        |
| 1     | N     | 6468:UNK  | C      | 6480:UNK  | N      | 27.60        |
| 1     | M     | 8442:UNK  | C      | 8449:UNK  | N      | 26.57        |
| 1     | N     | 8442:UNK  | C      | 8449:UNK  | N      | 26.57        |
| 1     | M     | 4325:UNK  | C      | 4337:UNK  | N      | 26.47        |
| 1     | N     | 4325:UNK  | C      | 4337:UNK  | N      | 26.46        |
| 1     | M     | 8106:UNK  | C      | 8109:UNK  | N      | 25.92        |
| 1     | N     | 8106:UNK  | C      | 8109:UNK  | N      | 25.92        |
| 1     | M     | 6283:UNK  | C      | 6296:UNK  | N      | 25.90        |
| 1     | N     | 6283:UNK  | C      | 6296:UNK  | N      | 25.90        |
| 1     | M     | 292:UNK   | C      | 303:UNK   | N      | 25.77        |
| 1     | N     | 292:UNK   | C      | 303:UNK   | N      | 25.77        |
| 1     | M     | 8483:UNK  | C      | 8485:UNK  | N      | 24.83        |
| 1     | N     | 8483:UNK  | C      | 8485:UNK  | N      | 24.83        |
| 1     | M     | 4875:UNK  | C      | 4886:UNK  | N      | 24.81        |
| 1     | N     | 4875:UNK  | C      | 4886:UNK  | N      | 24.81        |
| 1     | M     | 186:UNK   | C      | 200:UNK   | N      | 24.57        |
| 1     | N     | 186:UNK   | C      | 200:UNK   | N      | 24.57        |
| 1     | M     | 4540:UNK  | C      | 4552:UNK  | N      | 24.41        |
| 1     | N     | 4540:UNK  | C      | 4552:UNK  | N      | 24.41        |
| 1     | M     | 5211:UNK  | C      | 5225:UNK  | N      | 24.30        |
| 1     | M     | 8325:UNK  | C      | 8338:UNK  | N      | 24.29        |
| 1     | N     | 5211:UNK  | C      | 5225:UNK  | N      | 24.29        |
| 1     | N     | 8325:UNK  | C      | 8338:UNK  | N      | 24.29        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 134:UNK   | C      | 138:UNK   | N      | 23.96        |
| 1     | M     | 350:UNK   | C      | 365:UNK   | N      | 23.96        |
| 1     | N     | 134:UNK   | C      | 138:UNK   | N      | 23.96        |
| 1     | N     | 350:UNK   | C      | 365:UNK   | N      | 23.96        |
| 1     | M     | 6711:UNK  | C      | 6724:UNK  | N      | 23.79        |
| 1     | N     | 6711:UNK  | C      | 6724:UNK  | N      | 23.79        |
| 1     | M     | 6845:UNK  | C      | 6856:UNK  | N      | 23.48        |
| 1     | N     | 6845:UNK  | C      | 6856:UNK  | N      | 23.48        |
| 1     | M     | 6935:UNK  | C      | 7068:UNK  | N      | 23.38        |
| 1     | N     | 6935:UNK  | C      | 7068:UNK  | N      | 23.38        |
| 1     | M     | 4931:UNK  | C      | 4942:UNK  | N      | 23.35        |
| 1     | N     | 4931:UNK  | C      | 4942:UNK  | N      | 23.35        |
| 1     | M     | 2558:UNK  | C      | 2569:UNK  | N      | 23.23        |
| 1     | N     | 2558:UNK  | C      | 2569:UNK  | N      | 23.23        |
| 1     | M     | 8156:UNK  | C      | 8166:UNK  | N      | 23.07        |
| 1     | N     | 8156:UNK  | C      | 8166:UNK  | N      | 23.07        |
| 1     | M     | 6350:UNK  | C      | 6372:UNK  | N      | 22.69        |
| 1     | N     | 6350:UNK  | C      | 6372:UNK  | N      | 22.69        |
| 1     | M     | 4417:UNK  | C      | 4431:UNK  | N      | 22.67        |
| 1     | N     | 4417:UNK  | C      | 4431:UNK  | N      | 22.67        |
| 1     | M     | 117:UNK   | C      | 119:UNK   | N      | 22.35        |
| 1     | N     | 117:UNK   | C      | 119:UNK   | N      | 22.35        |
| 1     | M     | 4380:UNK  | C      | 4386:UNK  | N      | 21.94        |
| 1     | N     | 4380:UNK  | C      | 4386:UNK  | N      | 21.94        |
| 1     | M     | 4644:UNK  | C      | 4671:UNK  | N      | 21.42        |
| 1     | N     | 4644:UNK  | C      | 4671:UNK  | N      | 21.42        |
| 1     | M     | 6888:UNK  | C      | 6900:UNK  | N      | 20.85        |
| 1     | N     | 6888:UNK  | C      | 6900:UNK  | N      | 20.85        |
| 1     | M     | 8427:UNK  | C      | 8432:UNK  | N      | 20.71        |
| 1     | N     | 8427:UNK  | C      | 8432:UNK  | N      | 20.71        |
| 1     | M     | 264:UNK   | C      | 276:UNK   | N      | 20.62        |
| 1     | N     | 264:UNK   | C      | 276:UNK   | N      | 20.62        |
| 1     | M     | 63:UNK    | C      | 69:UNK    | N      | 20.54        |
| 1     | N     | 63:UNK    | C      | 69:UNK    | N      | 20.54        |
| 1     | M     | 17:UNK    | C      | 24:UNK    | N      | 20.40        |
| 1     | N     | 17:UNK    | C      | 24:UNK    | N      | 20.40        |
| 1     | M     | 150:UNK   | C      | 158:UNK   | N      | 19.85        |
| 1     | N     | 150:UNK   | C      | 158:UNK   | N      | 19.85        |
| 1     | M     | 4950:UNK  | C      | 5137:UNK  | N      | 19.70        |
| 1     | N     | 4950:UNK  | C      | 5137:UNK  | N      | 19.70        |
| 1     | M     | 4794:UNK  | C      | 4804:UNK  | N      | 19.52        |
| 1     | N     | 4794:UNK  | C      | 4804:UNK  | N      | 19.52        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 8204:UNK  | C      | 8211:UNK  | N      | 19.44        |
| 1     | N     | 8204:UNK  | C      | 8211:UNK  | N      | 19.43        |
| 1     | M     | 4399:UNK  | C      | 4407:UNK  | N      | 19.41        |
| 1     | N     | 4399:UNK  | C      | 4407:UNK  | N      | 19.41        |
| 1     | M     | 4163:UNK  | C      | 4173:UNK  | N      | 19.34        |
| 1     | N     | 4163:UNK  | C      | 4173:UNK  | N      | 19.34        |
| 1     | M     | 2647:UNK  | C      | 2663:UNK  | N      | 19.24        |
| 1     | N     | 2647:UNK  | C      | 2663:UNK  | N      | 19.24        |
| 1     | M     | 98:UNK    | C      | 108:UNK   | N      | 19.08        |
| 1     | N     | 98:UNK    | C      | 108:UNK   | N      | 19.08        |
| 1     | M     | 4854:UNK  | C      | 4865:UNK  | N      | 19.05        |
| 1     | N     | 4854:UNK  | C      | 4865:UNK  | N      | 19.05        |
| 1     | M     | 6557:UNK  | C      | 6601:UNK  | N      | 18.71        |
| 1     | N     | 6557:UNK  | C      | 6601:UNK  | N      | 18.71        |
| 1     | M     | 6911:UNK  | C      | 6924:UNK  | N      | 18.05        |
| 1     | N     | 6911:UNK  | C      | 6924:UNK  | N      | 18.05        |
| 1     | M     | 2809:UNK  | C      | 2822:UNK  | N      | 17.92        |
| 1     | N     | 2809:UNK  | C      | 2822:UNK  | N      | 17.92        |
| 1     | N     | 4828:UNK  | C      | 4841:UNK  | N      | 17.16        |
| 1     | M     | 4828:UNK  | C      | 4841:UNK  | N      | 17.15        |
| 1     | M     | 8179:UNK  | C      | 8193:UNK  | N      | 17.14        |
| 1     | N     | 8179:UNK  | C      | 8193:UNK  | N      | 17.14        |
| 1     | M     | 6194:UNK  | C      | 6210:UNK  | N      | 15.76        |
| 1     | N     | 6194:UNK  | C      | 6210:UNK  | N      | 15.76        |
| 1     | B     | 254:UNK   | C      | 261:UNK   | N      | 15.57        |
| 1     | D     | 254:UNK   | C      | 261:UNK   | N      | 15.57        |
| 1     | M     | 382:UNK   | C      | 394:UNK   | N      | 15.53        |
| 1     | N     | 382:UNK   | C      | 394:UNK   | N      | 15.53        |
| 1     | M     | 6161:UNK  | C      | 6172:UNK  | N      | 15.30        |
| 1     | N     | 6161:UNK  | C      | 6172:UNK  | N      | 15.30        |
| 1     | M     | 79:UNK    | C      | 83:UNK    | N      | 15.14        |
| 1     | N     | 79:UNK    | C      | 83:UNK    | N      | 15.14        |
| 1     | M     | 8355:UNK  | C      | 8367:UNK  | N      | 15.11        |
| 1     | N     | 8355:UNK  | C      | 8367:UNK  | N      | 15.11        |
| 1     | M     | 6416:UNK  | C      | 6431:UNK  | N      | 14.90        |
| 1     | N     | 6416:UNK  | C      | 6431:UNK  | N      | 14.90        |
| 1     | N     | 7167:UNK  | C      | 7201:UNK  | N      | 14.22        |
| 1     | M     | 7167:UNK  | C      | 7201:UNK  | N      | 14.21        |
| 1     | M     | 8269:UNK  | C      | 8274:UNK  | N      | 14.20        |
| 1     | N     | 8269:UNK  | C      | 8274:UNK  | N      | 14.20        |
| 1     | M     | 442:UNK   | C      | 455:UNK   | N      | 14.03        |
| 1     | N     | 442:UNK   | C      | 455:UNK   | N      | 14.03        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 4128:UNK  | C      | 4136:UNK  | N      | 14.01        |
| 1     | N     | 4128:UNK  | C      | 4136:UNK  | N      | 14.01        |
| 1     | M     | 6316:UNK  | C      | 6327:UNK  | N      | 13.82        |
| 1     | N     | 6316:UNK  | C      | 6327:UNK  | N      | 13.82        |
| 1     | M     | 38:UNK    | C      | 44:UNK    | N      | 13.50        |
| 1     | N     | 38:UNK    | C      | 44:UNK    | N      | 13.50        |
| 1     | B     | 84:UNK    | C      | 91:UNK    | N      | 12.91        |
| 1     | D     | 84:UNK    | C      | 91:UNK    | N      | 12.91        |
| 1     | M     | 2608:UNK  | C      | 2630:UNK  | N      | 12.79        |
| 1     | N     | 2608:UNK  | C      | 2630:UNK  | N      | 12.79        |
| 1     | B     | 42:UNK    | C      | 49:UNK    | N      | 12.40        |
| 1     | D     | 42:UNK    | C      | 49:UNK    | N      | 12.40        |
| 1     | M     | 6532:UNK  | C      | 6542:UNK  | N      | 12.09        |
| 1     | N     | 6532:UNK  | C      | 6542:UNK  | N      | 12.09        |
| 1     | M     | 4588:UNK  | C      | 4598:UNK  | N      | 11.91        |
| 1     | N     | 4588:UNK  | C      | 4598:UNK  | N      | 11.90        |
| 1     | B     | 168:UNK   | C      | 175:UNK   | N      | 11.88        |
| 1     | D     | 168:UNK   | C      | 175:UNK   | N      | 11.88        |
| 1     | M     | 6622:UNK  | C      | 6636:UNK  | N      | 11.62        |
| 1     | N     | 6622:UNK  | C      | 6636:UNK  | N      | 11.61        |
| 1     | M     | 6242:UNK  | C      | 6267:UNK  | N      | 11.55        |
| 1     | N     | 6242:UNK  | C      | 6267:UNK  | N      | 11.55        |
| 1     | M     | 8407:UNK  | C      | 8415:UNK  | N      | 11.17        |
| 1     | N     | 8407:UNK  | C      | 8415:UNK  | N      | 11.16        |
| 1     | N     | 4303:UNK  | C      | 4314:UNK  | N      | 11.14        |
| 1     | M     | 4303:UNK  | C      | 4314:UNK  | N      | 11.13        |
| 1     | B     | 127:UNK   | C      | 133:UNK   | N      | 11.04        |
| 1     | D     | 127:UNK   | C      | 133:UNK   | N      | 11.04        |
| 1     | M     | 4499:UNK  | C      | 4511:UNK  | N      | 10.80        |
| 1     | N     | 4499:UNK  | C      | 4511:UNK  | N      | 10.80        |
| 1     | M     | 8379:UNK  | C      | 8393:UNK  | N      | 10.75        |
| 1     | N     | 8379:UNK  | C      | 8393:UNK  | N      | 10.75        |
| 1     | M     | 5262:UNK  | C      | 5273:UNK  | N      | 10.22        |
| 1     | N     | 5262:UNK  | C      | 5273:UNK  | N      | 10.22        |
| 1     | B     | 211:UNK   | C      | 216:UNK   | N      | 10.20        |
| 1     | D     | 211:UNK   | C      | 216:UNK   | N      | 10.20        |
| 1     | M     | 6389:UNK  | C      | 6402:UNK  | N      | 10.15        |
| 1     | N     | 6389:UNK  | C      | 6402:UNK  | N      | 10.15        |
| 1     | M     | 319:UNK   | C      | 332:UNK   | N      | 10.11        |
| 1     | N     | 319:UNK   | C      | 332:UNK   | N      | 10.11        |
| 1     | M     | 169:UNK   | C      | 175:UNK   | N      | 10.01        |
| 1     | N     | 169:UNK   | C      | 175:UNK   | N      | 10.01        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 8460:UNK  | C      | 8471:UNK  | N      | 9.97         |
| 1     | N     | 8460:UNK  | C      | 8471:UNK  | N      | 9.97         |
| 1     | M     | 7143:UNK  | C      | 7147:UNK  | N      | 9.83         |
| 1     | N     | 7143:UNK  | C      | 7147:UNK  | N      | 9.83         |
| 1     | B     | 299:UNK   | C      | 304:UNK   | N      | 9.31         |
| 1     | D     | 299:UNK   | C      | 304:UNK   | N      | 9.31         |
| 1     | M     | 4145:UNK  | C      | 4151:UNK  | N      | 8.71         |
| 1     | N     | 4145:UNK  | C      | 4151:UNK  | N      | 8.71         |
| 1     | M     | 6442:UNK  | C      | 6453:UNK  | N      | 8.69         |
| 1     | N     | 6442:UNK  | C      | 6453:UNK  | N      | 8.69         |
| 1     | B     | 320:UNK   | C      | 327:UNK   | N      | 7.11         |
| 1     | D     | 320:UNK   | C      | 327:UNK   | N      | 7.11         |
| 1     | B     | 97:UNK    | C      | 101:UNK   | N      | 7.02         |
| 1     | D     | 97:UNK    | C      | 101:UNK   | N      | 7.02         |
| 1     | N     | 4525:UNK  | C      | 4529:UNK  | N      | 6.93         |
| 1     | M     | 4525:UNK  | C      | 4529:UNK  | N      | 6.92         |
| 1     | B     | 287:UNK   | C      | 293:UNK   | N      | 6.66         |
| 1     | D     | 287:UNK   | C      | 293:UNK   | N      | 6.66         |
| 1     | B     | 199:UNK   | C      | 205:UNK   | N      | 6.62         |
| 1     | D     | 199:UNK   | C      | 205:UNK   | N      | 6.62         |
| 1     | B     | 179:UNK   | C      | 184:UNK   | N      | 6.48         |
| 1     | D     | 179:UNK   | C      | 184:UNK   | N      | 6.48         |
| 1     | B     | 309:UNK   | C      | 315:UNK   | N      | 5.88         |
| 1     | D     | 309:UNK   | C      | 315:UNK   | N      | 5.88         |
| 1     | B     | 268:UNK   | C      | 272:UNK   | N      | 5.87         |
| 1     | D     | 268:UNK   | C      | 272:UNK   | N      | 5.86         |
| 1     | B     | 222:UNK   | C      | 228:UNK   | N      | 5.63         |
| 1     | D     | 222:UNK   | C      | 228:UNK   | N      | 5.63         |
| 1     | B     | 138:UNK   | C      | 142:UNK   | N      | 5.56         |
| 1     | D     | 138:UNK   | C      | 142:UNK   | N      | 5.56         |
| 1     | B     | 277:UNK   | C      | 283:UNK   | N      | 5.52         |
| 1     | D     | 277:UNK   | C      | 283:UNK   | N      | 5.52         |
| 1     | B     | 54:UNK    | C      | 58:UNK    | N      | 5.34         |
| 1     | D     | 54:UNK    | C      | 58:UNK    | N      | 5.34         |
| 1     | B     | 157:UNK   | C      | 162:UNK   | N      | 4.74         |
| 1     | D     | 157:UNK   | C      | 162:UNK   | N      | 4.74         |
| 1     | B     | 233:UNK   | C      | 237:UNK   | N      | 4.70         |
| 1     | D     | 233:UNK   | C      | 237:UNK   | N      | 4.70         |
| 1     | B     | 73:UNK    | C      | 78:UNK    | N      | 4.64         |
| 1     | D     | 73:UNK    | C      | 78:UNK    | N      | 4.64         |
| 1     | B     | 64:UNK    | C      | 67:UNK    | N      | 3.96         |
| 1     | D     | 64:UNK    | C      | 67:UNK    | N      | 3.96         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 8287:UNK  | C      | 8289:UNK  | N      | 3.95         |
| 1     | N     | 8287:UNK  | C      | 8289:UNK  | N      | 3.95         |
| 1     | B     | 106:UNK   | C      | 109:UNK   | N      | 3.94         |
| 1     | D     | 106:UNK   | C      | 109:UNK   | N      | 3.94         |
| 1     | B     | 242:UNK   | C      | 246:UNK   | N      | 3.91         |
| 1     | D     | 242:UNK   | C      | 246:UNK   | N      | 3.91         |
| 1     | B     | 190:UNK   | C      | 193:UNK   | N      | 3.80         |
| 1     | D     | 190:UNK   | C      | 193:UNK   | N      | 3.80         |
| 1     | B     | 148:UNK   | C      | 151:UNK   | N      | 3.75         |
| 1     | D     | 148:UNK   | C      | 151:UNK   | N      | 3.74         |
| 1     | B     | 116:UNK   | C      | 119:UNK   | N      | 3.73         |
| 1     | D     | 116:UNK   | C      | 119:UNK   | N      | 3.73         |



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2 |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------|-------|-----------------------|-------|
| 1   | A     | 374/446 (83%)  | 0.57   | 33 (8%) | 10 12 | 200, 200, 200, 200    | 0     |
| 1   | C     | 374/446 (83%)  | 0.42   | 23 (6%) | 21 20 | 200, 200, 200, 200    | 0     |
| 2   | B     | 0/400          | -      | -       |       | -                     | -     |
| 2   | D     | 0/400          | -      | -       |       | -                     | -     |
| 3   | M     | 0/2300         | -      | -       |       | -                     | -     |
| 3   | N     | 0/2300         | -      | -       |       | -                     | -     |
| All | All   | 748/6292 (11%) | 0.49   | 56 (7%) | 14 15 | 200, 200, 200, 200    | 0     |

All (56) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 108 | SER  | 5.3  |
| 1   | A     | 384 | THR  | 5.3  |
| 1   | A     | 106 | ALA  | 5.2  |
| 1   | C     | 335 | THR  | 4.7  |
| 1   | A     | 104 | CYS  | 4.5  |
| 1   | A     | 424 | GLU  | 4.3  |
| 1   | C     | 390 | TYR  | 4.1  |
| 1   | C     | 283 | GLN  | 4.0  |
| 1   | A     | 267 | GLU  | 3.9  |
| 1   | A     | 305 | GLU  | 3.9  |
| 1   | C     | 399 | ARG  | 3.6  |
| 1   | A     | 435 | GLU  | 3.6  |
| 1   | A     | 386 | GLU  | 3.5  |
| 1   | A     | 411 | SER  | 3.5  |
| 1   | A     | 179 | LYS  | 3.5  |
| 1   | C     | 336 | VAL  | 3.3  |
| 1   | A     | 335 | THR  | 3.3  |
| 1   | A     | 105 | GLN  | 3.1  |
| 1   | A     | 304 | LEU  | 3.1  |
| 1   | C     | 394 | VAL  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 362 | SER  | 3.0  |
| 1   | C     | 398 | GLY  | 2.9  |
| 1   | C     | 397 | ALA  | 2.9  |
| 1   | A     | 248 | ALA  | 2.9  |
| 1   | C     | 302 | ASP  | 2.9  |
| 1   | A     | 286 | ILE  | 2.8  |
| 1   | C     | 337 | HIS  | 2.8  |
| 1   | C     | 395 | GLY  | 2.7  |
| 1   | A     | 287 | LYS  | 2.7  |
| 1   | A     | 385 | ASN  | 2.7  |
| 1   | A     | 397 | ALA  | 2.6  |
| 1   | A     | 107 | LYS  | 2.6  |
| 1   | A     | 368 | ARG  | 2.6  |
| 1   | C     | 108 | SER  | 2.5  |
| 1   | C     | 107 | LYS  | 2.5  |
| 1   | A     | 164 | VAL  | 2.5  |
| 1   | C     | 126 | PRO  | 2.5  |
| 1   | C     | 258 | CYS  | 2.4  |
| 1   | C     | 246 | PHE  | 2.4  |
| 1   | A     | 407 | ILE  | 2.4  |
| 1   | C     | 371 | ASP  | 2.4  |
| 1   | A     | 129 | GLY  | 2.3  |
| 1   | C     | 301 | LEU  | 2.3  |
| 1   | A     | 263 | GLN  | 2.3  |
| 1   | A     | 95  | GLN  | 2.3  |
| 1   | A     | 301 | LEU  | 2.3  |
| 1   | A     | 181 | LYS  | 2.2  |
| 1   | A     | 143 | ALA  | 2.1  |
| 1   | A     | 268 | ILE  | 2.1  |
| 1   | C     | 411 | SER  | 2.1  |
| 1   | A     | 433 | PHE  | 2.1  |
| 1   | C     | 111 | GLY  | 2.1  |
| 1   | A     | 410 | VAL  | 2.0  |
| 1   | A     | 250 | LEU  | 2.0  |
| 1   | C     | 140 | ARG  | 2.0  |
| 1   | C     | 396 | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

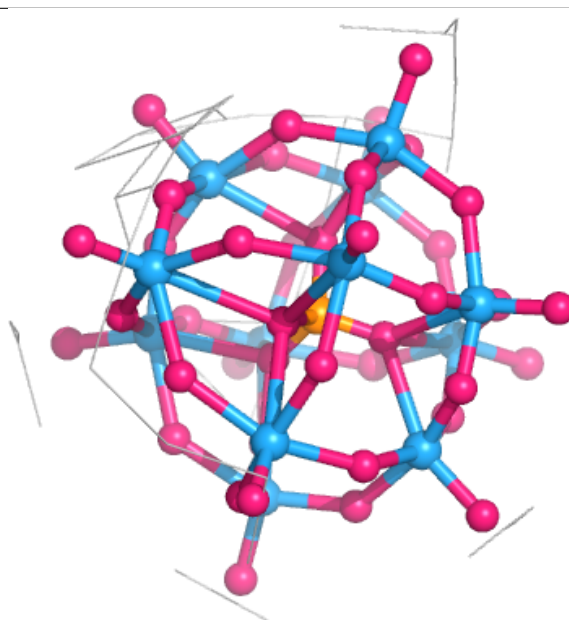
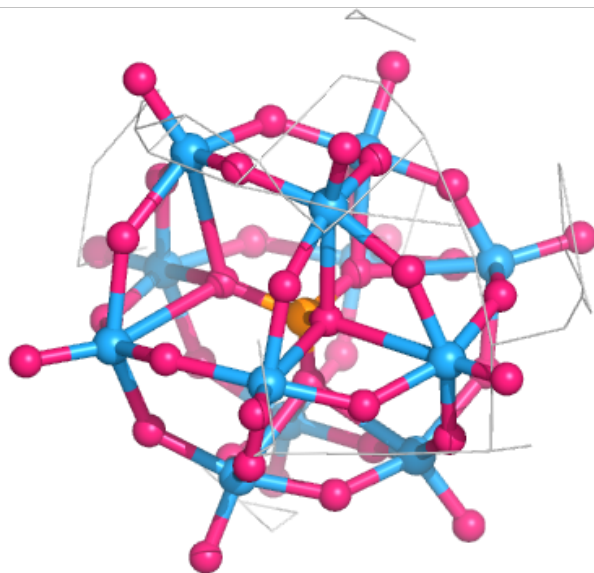
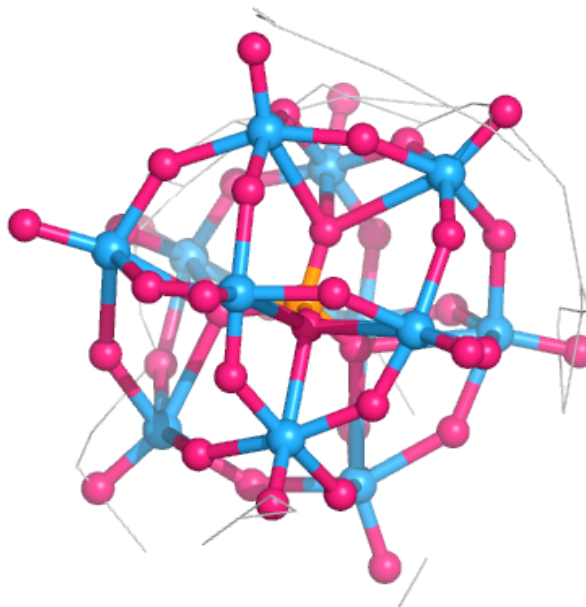
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | KEG  | A     | 503  | 53/53 | 0.87 | 0.35 | 200,200,200,200             | 53    |
| 4   | KEG  | A     | 502  | 53/53 | 0.88 | 0.25 | 200,200,200,200             | 53    |
| 4   | KEG  | N     | 8703 | 53/53 | 0.90 | 0.17 | 200,200,200,200             | 53    |
| 4   | KEG  | A     | 501  | 53/53 | 0.92 | 0.18 | 200,200,200,200             | 53    |
| 4   | KEG  | N     | 8702 | 53/53 | 0.97 | 0.15 | 200,200,200,200             | 53    |
| 4   | KEG  | N     | 8701 | 53/53 | 0.98 | 0.09 | 200,200,200,200             | 53    |
| 4   | KEG  | M     | 8701 | 53/53 | 0.98 | 0.16 | 200,200,200,200             | 53    |
| 4   | KEG  | M     | 8703 | 53/53 | 0.98 | 0.20 | 200,200,200,200             | 53    |
| 4   | KEG  | N     | 8704 | 53/53 | 0.98 | 0.16 | 200,200,200,200             | 53    |
| 4   | KEG  | N     | 8705 | 53/53 | 0.98 | 0.12 | 200,200,200,200             | 53    |
| 4   | KEG  | M     | 8702 | 53/53 | 0.99 | 0.09 | 200,200,200,200             | 53    |

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

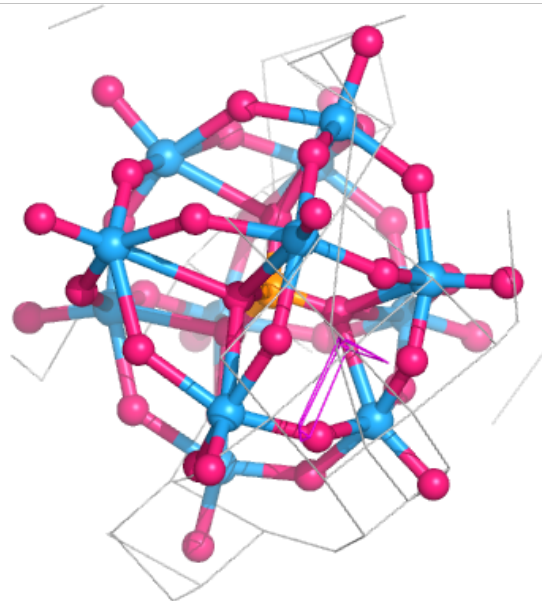
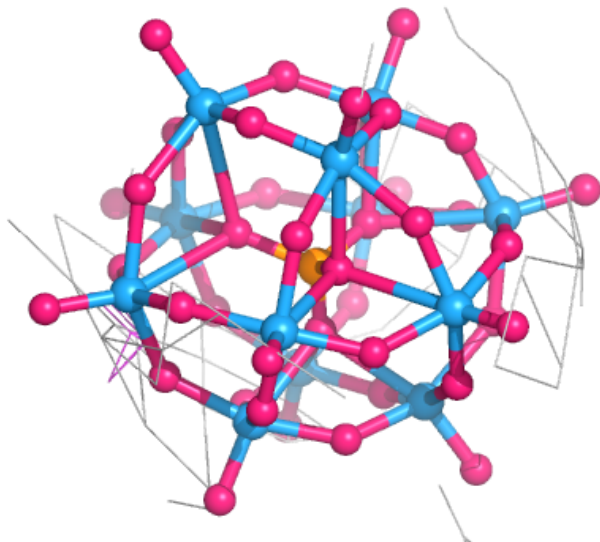
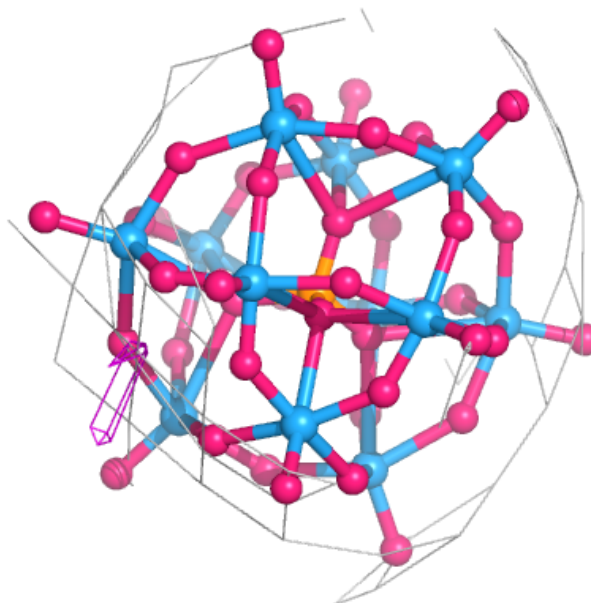
**Electron density around KEG A 503:**

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



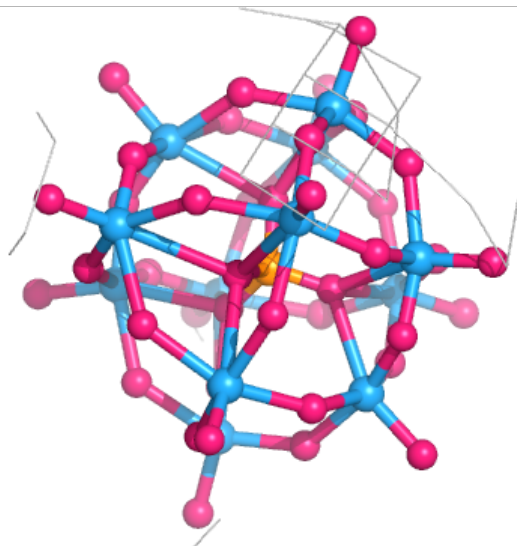
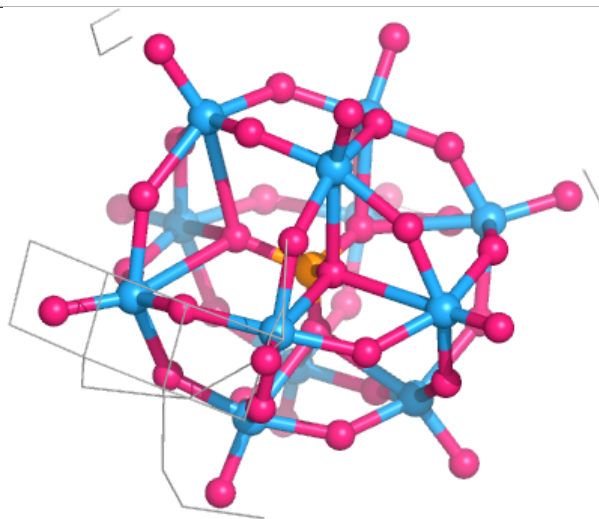
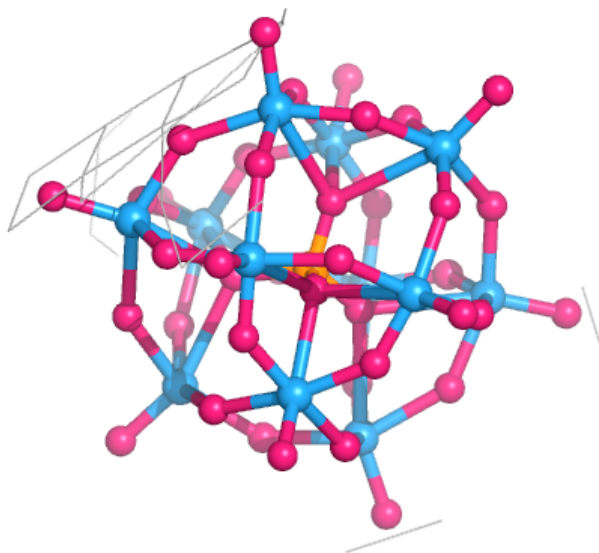
**Electron density around KEG A 502:**

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



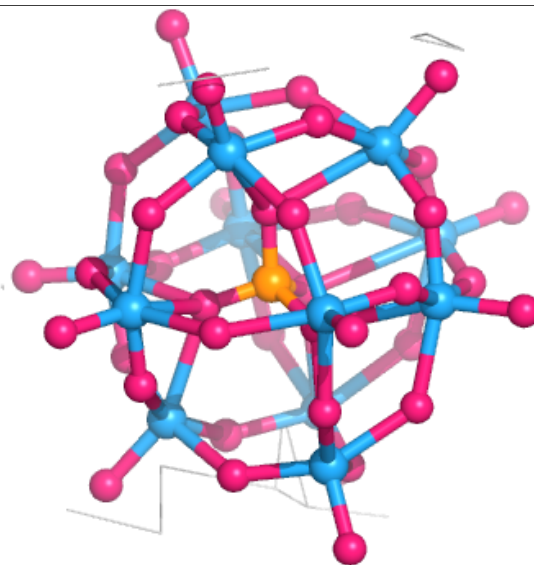
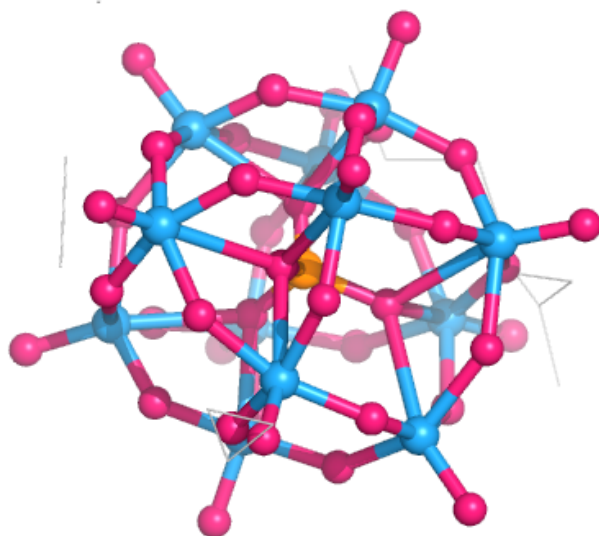
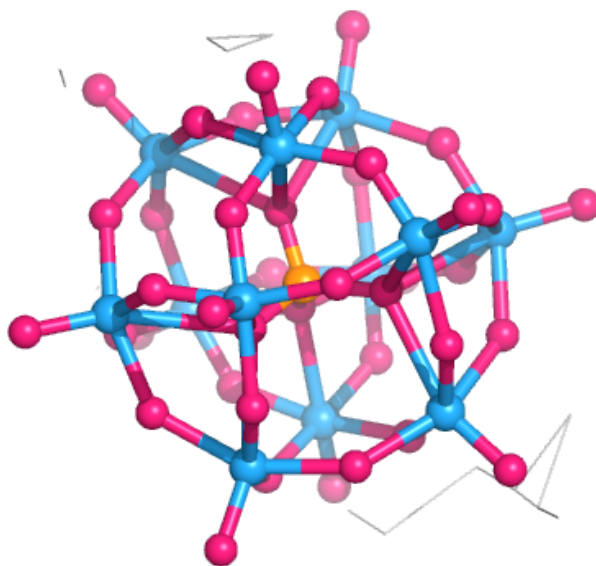
**Electron density around KEG N 8703:**

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



**Electron density around KEG A 501:**

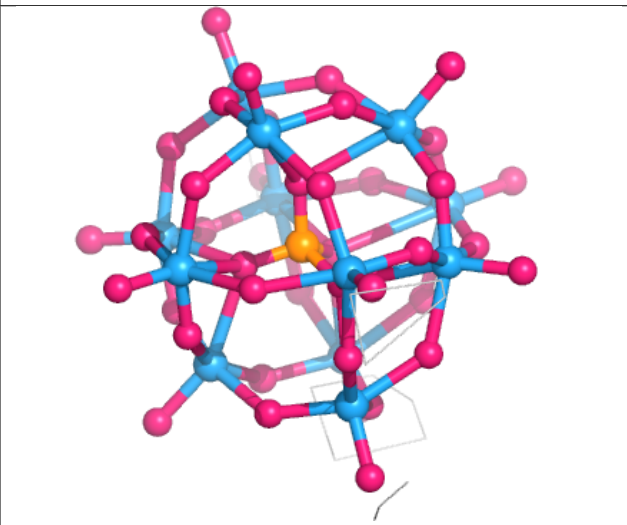
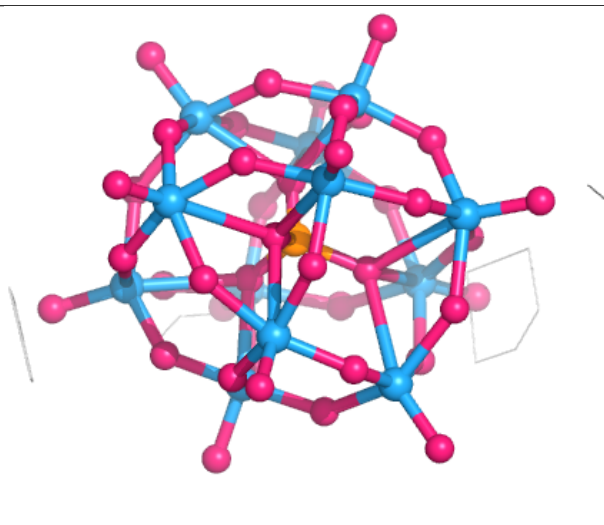
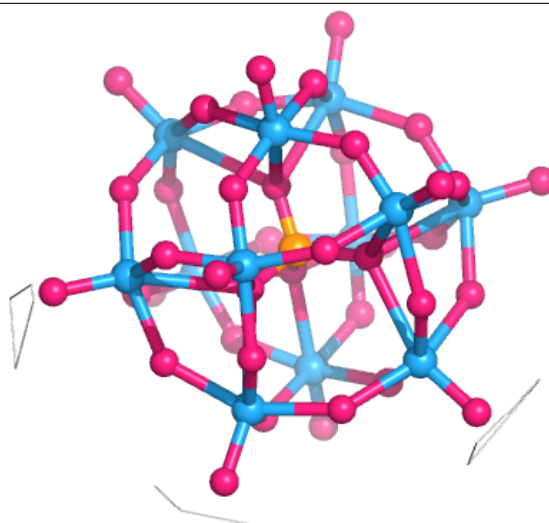
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around KEG N 8702:**

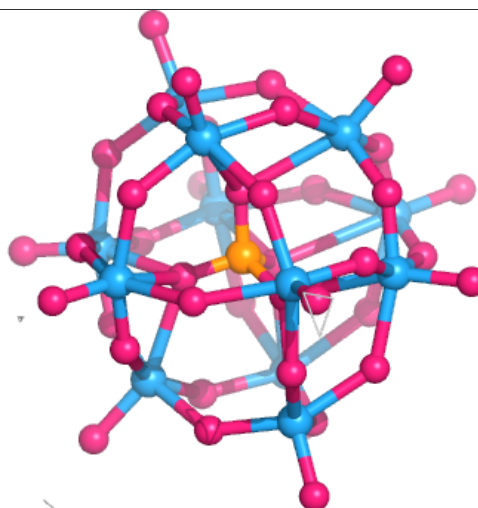
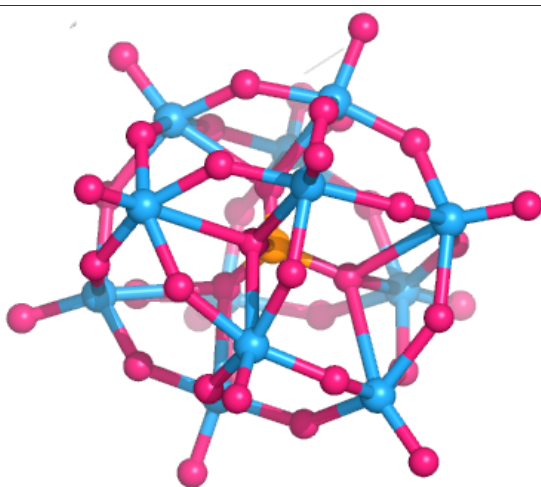
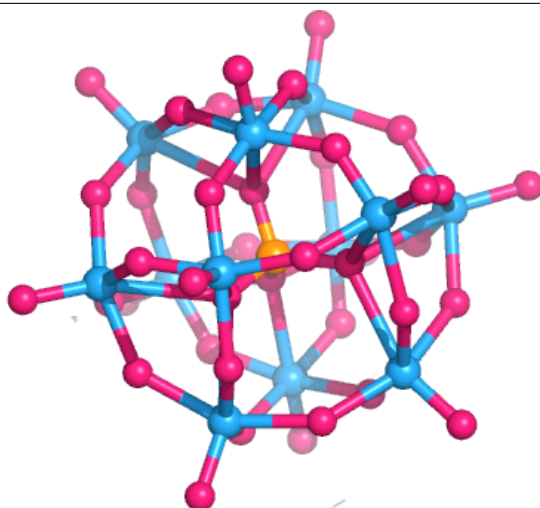
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





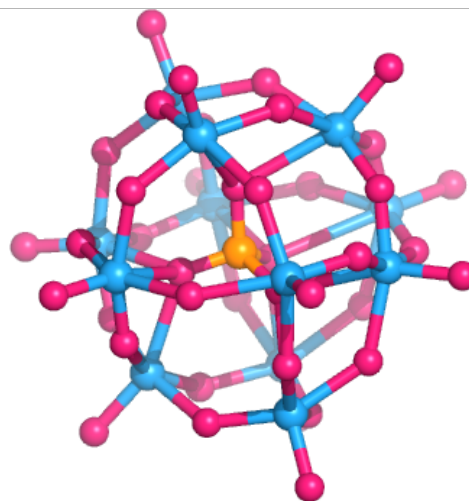
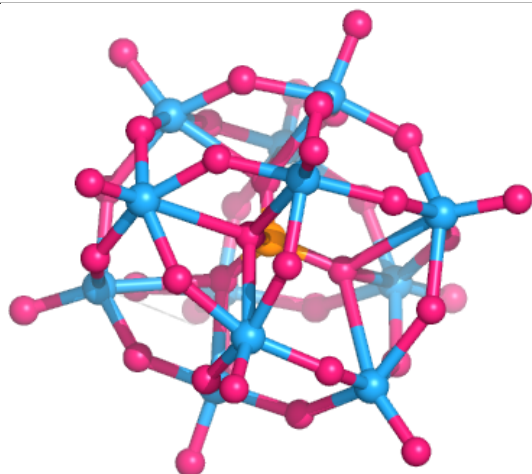
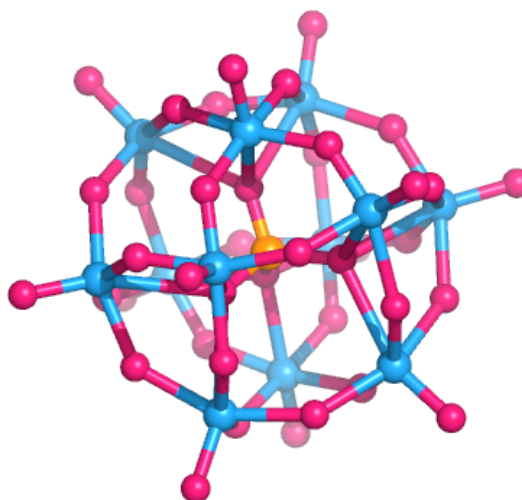
**Electron density around KEG N 8701:**

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



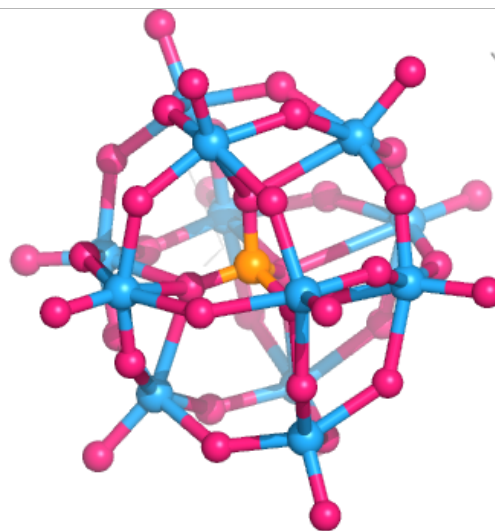
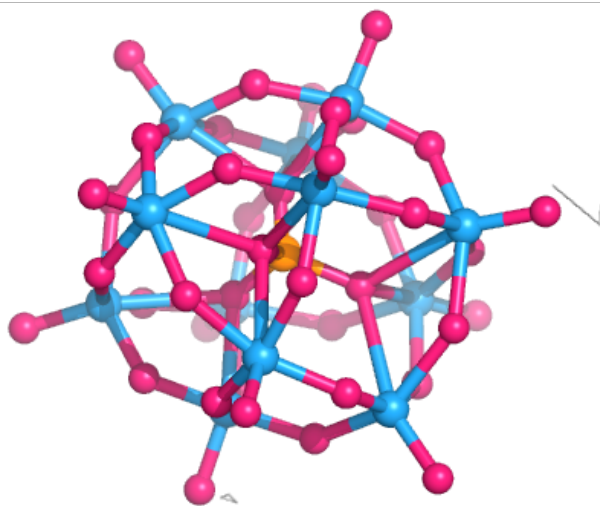
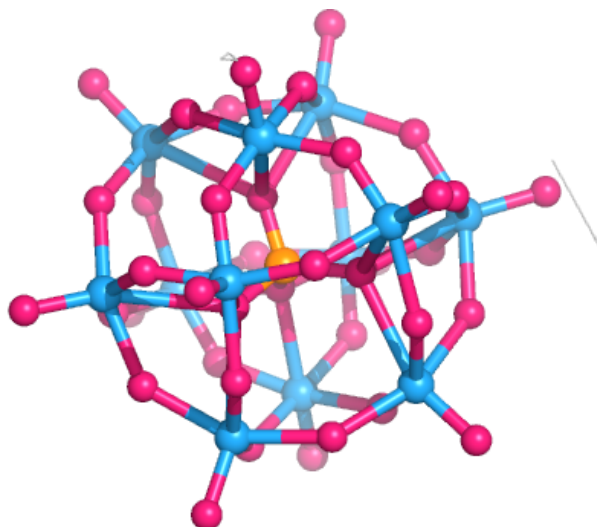
**Electron density around KEG M 8701:**

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



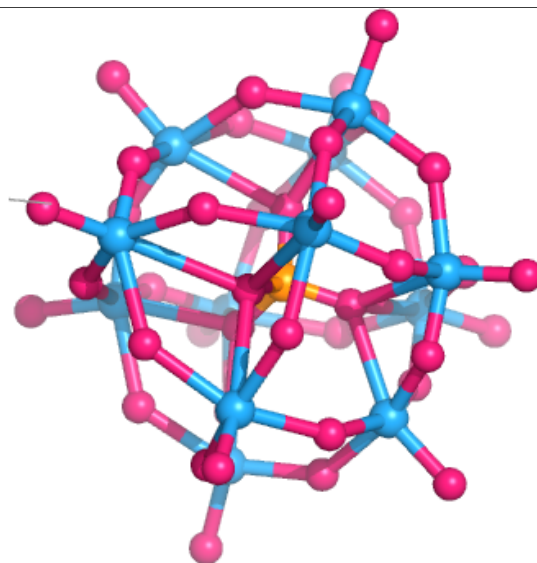
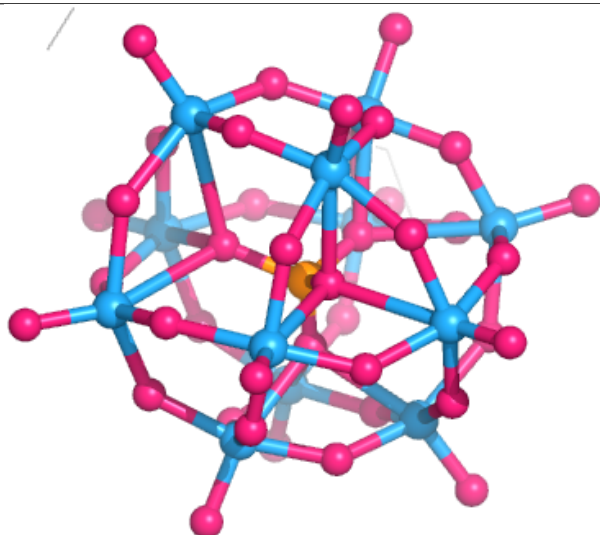
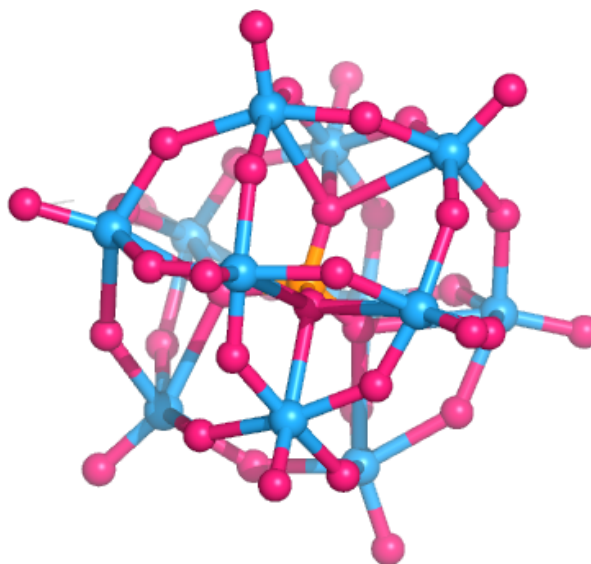
**Electron density around KEG M 8703:**

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



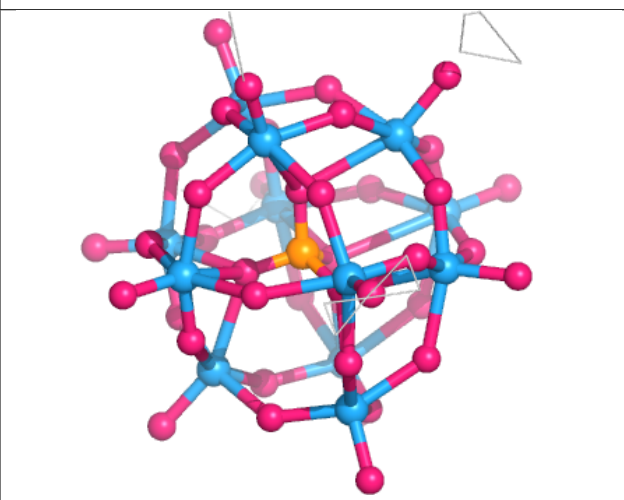
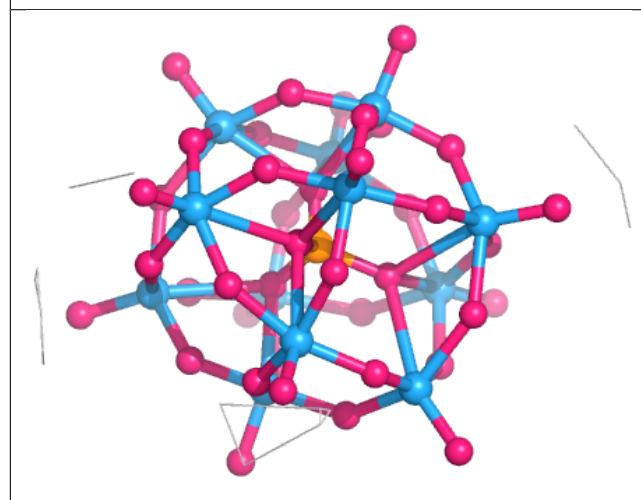
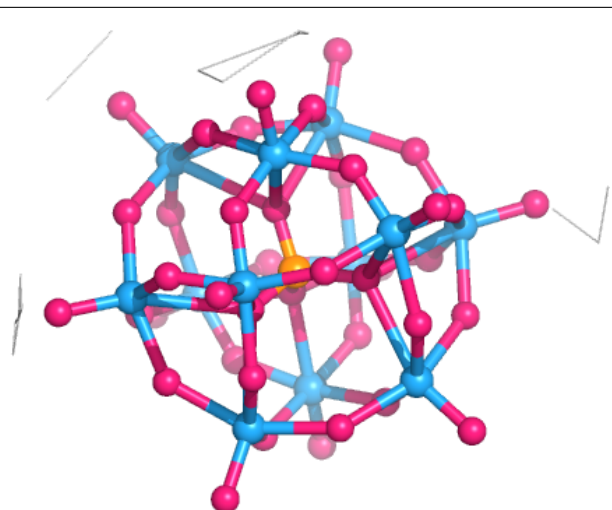
**Electron density around KEG N 8704:**

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



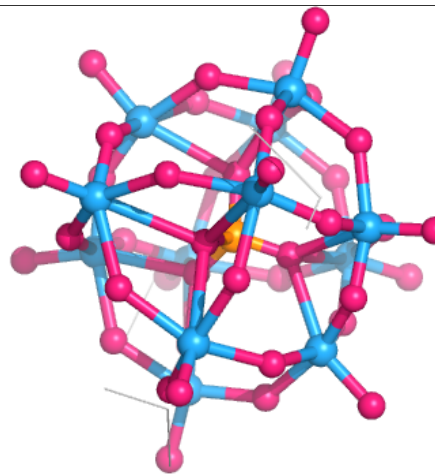
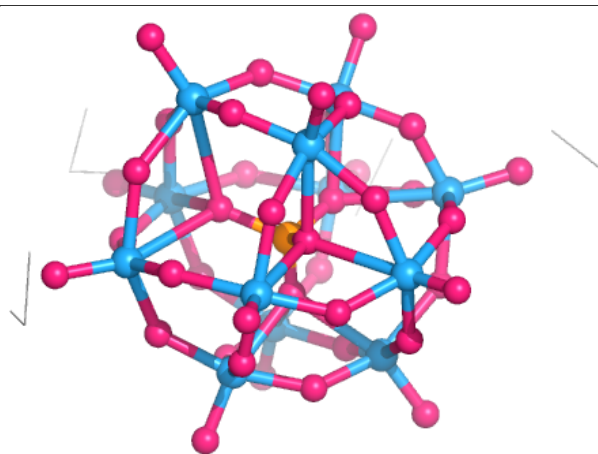
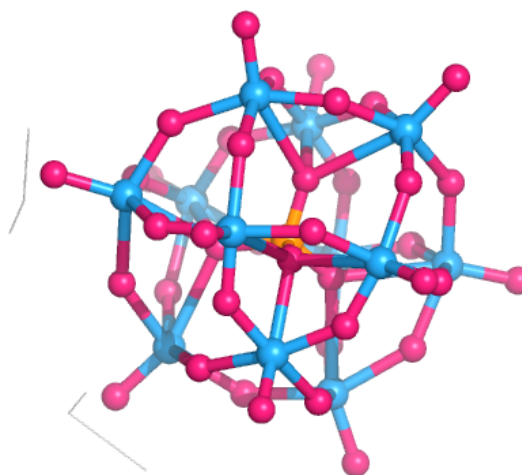
**Electron density around KEG N 8705:**

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



**Electron density around KEG M 8702:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.