# Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2026 – 01:59 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 6DHL / pdb_00006dhl |
| Title | : | Bovine glutamate dehydrogenase complexed with epicatechin-3-gallate (ECG) |
| Authors | : | Smith, T.J. |
| Deposited on | : | 2018-05-20 |
| Resolution | : | 3.62 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

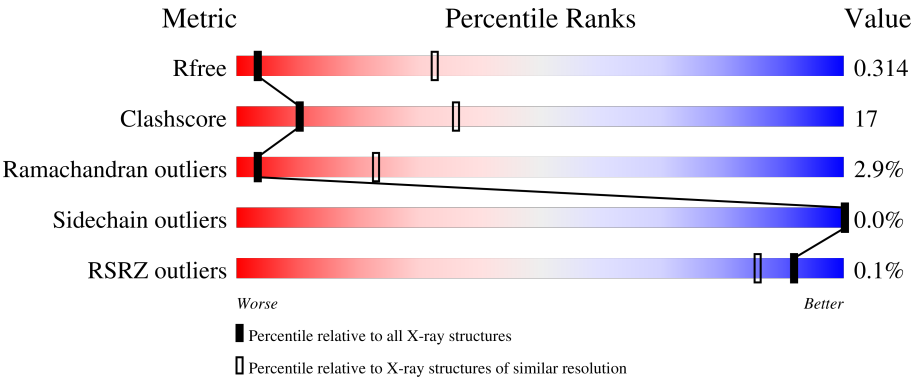
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.62 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 180053 | 1062 (3.72-3.52) |
| Clashscore | 190562 | 1092 (3.72-3.52) |
| Ramachandran outliers | 187476 | 1057 (3.72-3.52) |
| Sidechain outliers | 187428 | 1055 (3.72-3.52) |
| RSRZ outliers | 180081 | 1060 (3.72-3.52) |

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 >=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 <=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 | 496 | 65% 33% . |
| 1 | B | 496 | 64% 34% . |
| 1 | C | 496 | 67% 31% . |
| 1 | D | 496 | 64% 34% . |
| 1 | E | 496 | 61% 36% . |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 496 | 65% 33% |
| 1 | G | 496 | 61% 38% |
| 1 | H | 496 | 64% 35% |
| 1 | I | 496 | 64% 34% |
| 1 | J | 496 | 64% 34% |
| 1 | K | 496 | 63% 35% |
| 1 | L | 496 | 66% 33% |

## 2 Entry composition (i)

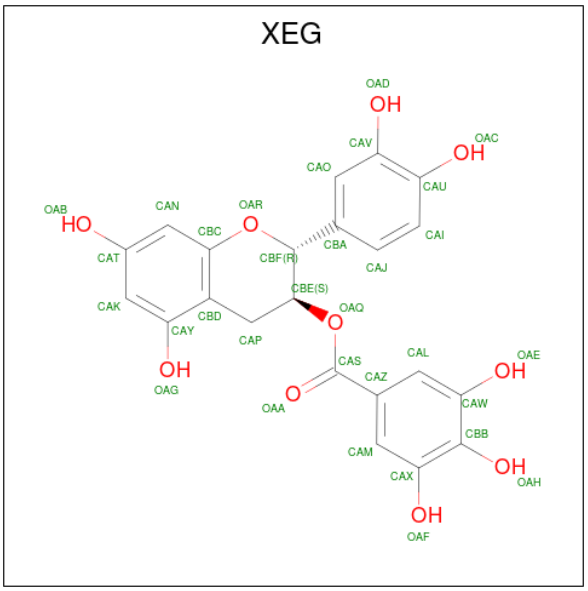
There are 2 unique types of molecules in this entry. The entry contains 46872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | B | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | C | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | D | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | E | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | F | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | G | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | H | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | I | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | J | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | K | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |
| 1 | L | 496 | Total 3874 | C 2451 | N 679 | O 725 | S 19 | 0 | 0 | 0 |

- Molecule 2 is (2R,3S)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3,4-dihydro-2H-chromen-3-yl 3,4,5-trihydroxybenzoate (CCD ID: XEG) (formula: $C_{22}H_{18}O_{10}$).



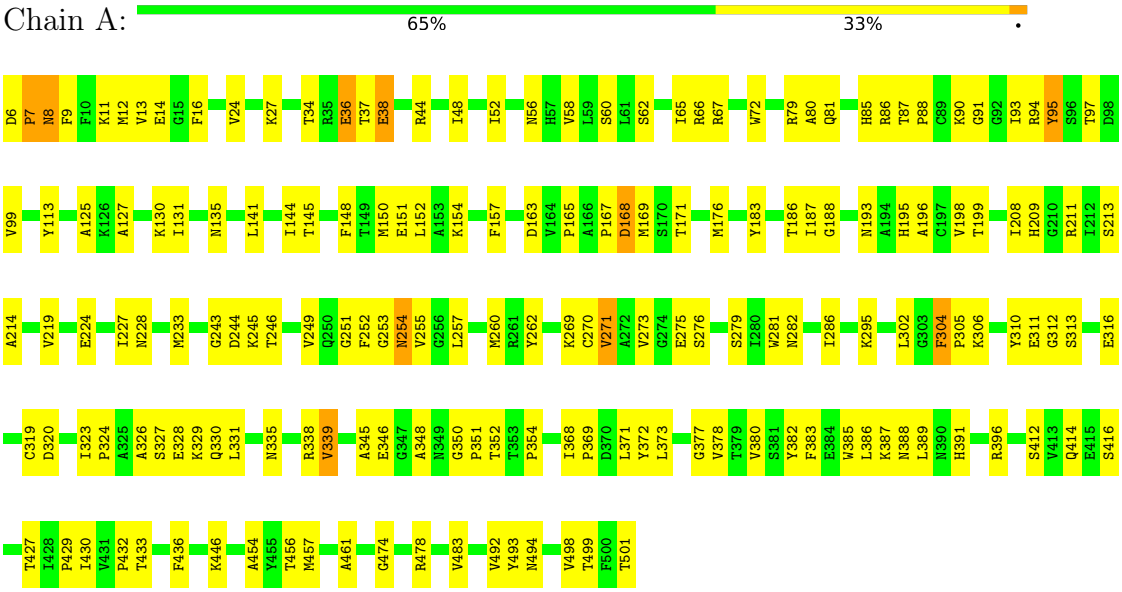

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | B | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | C | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | D | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | E | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | F | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | G | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | H | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | I | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | J | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | K | 1 | Total C O<br>32 22 10 | 0 | 0 |
| 2 | L | 1 | Total C O<br>32 22 10 | 0 | 0 |

# 3 Residue-property plots (i)

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.

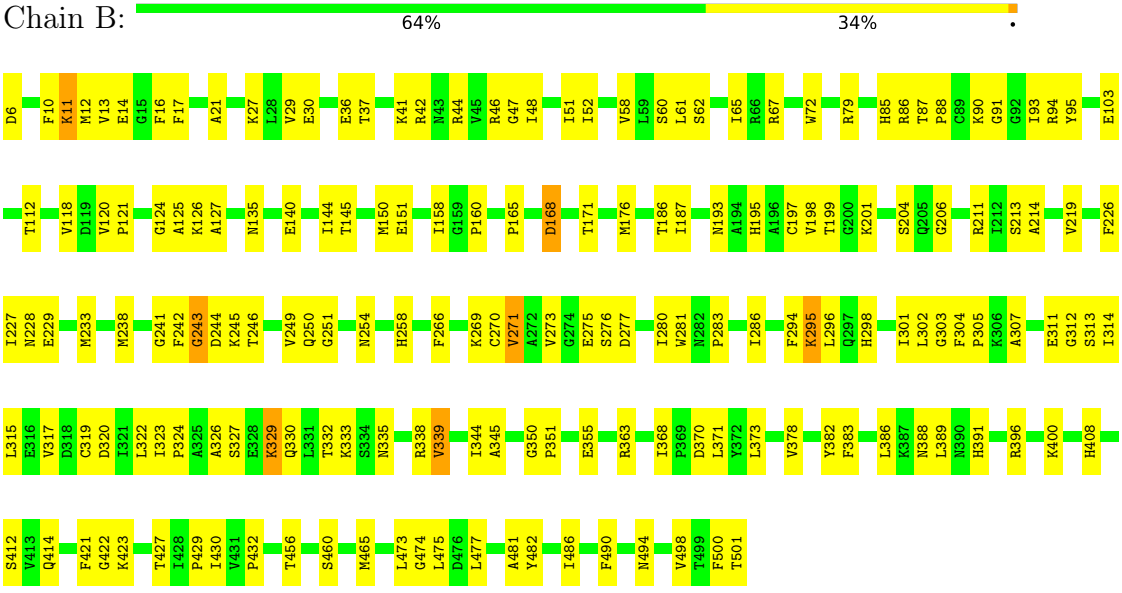
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain A:



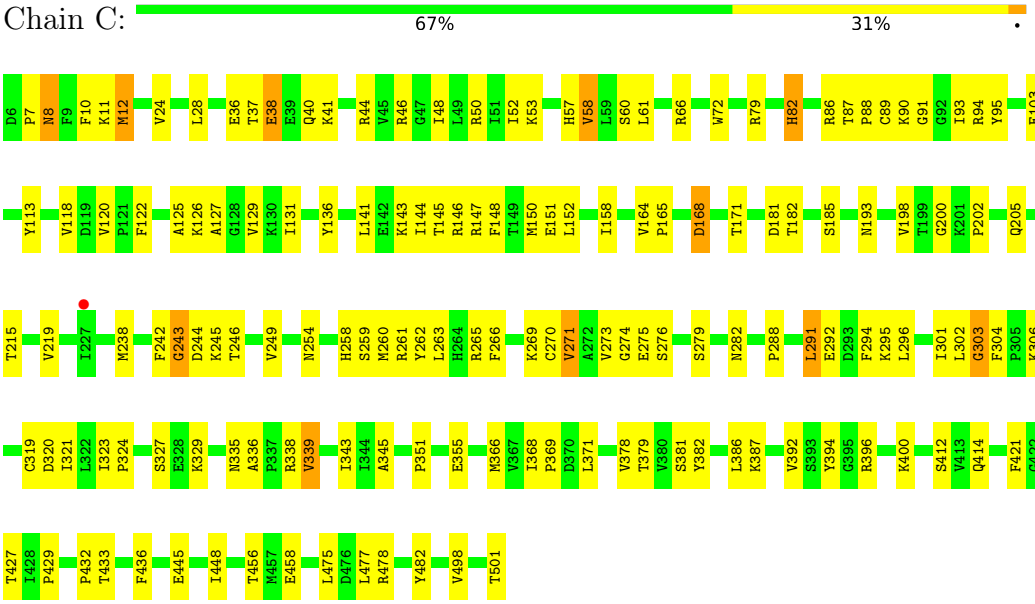

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain B:



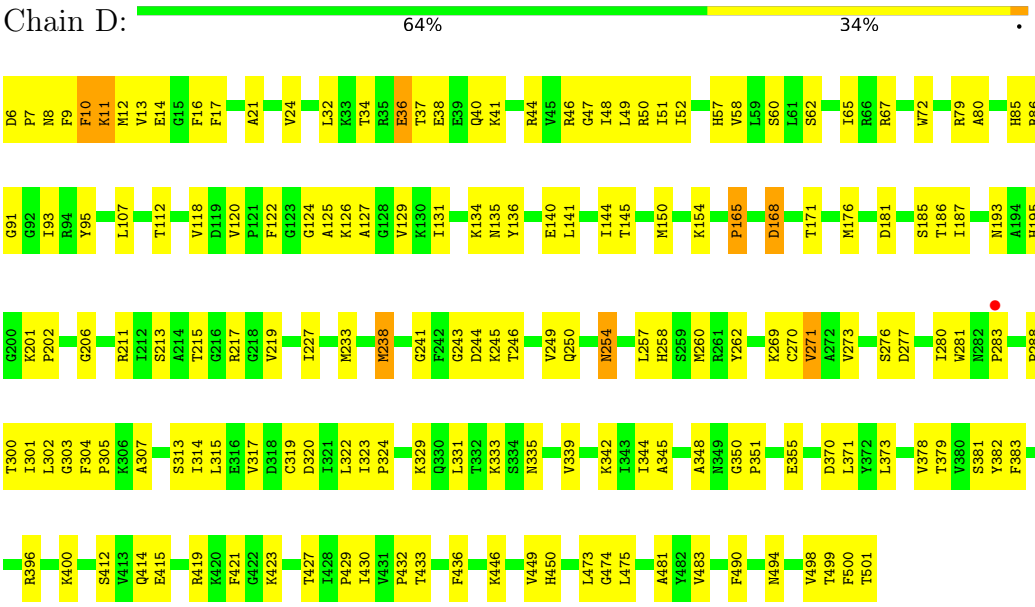
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:



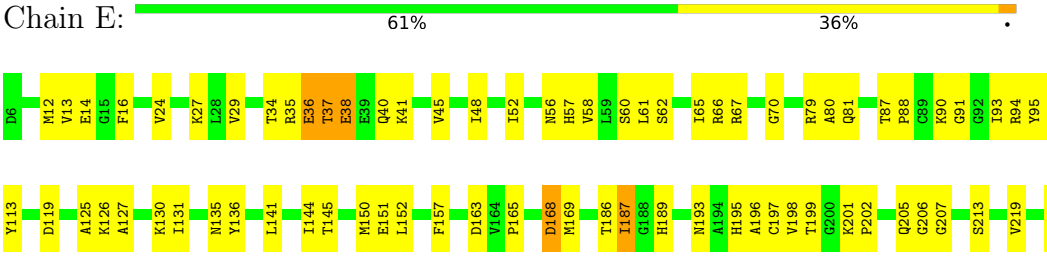

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

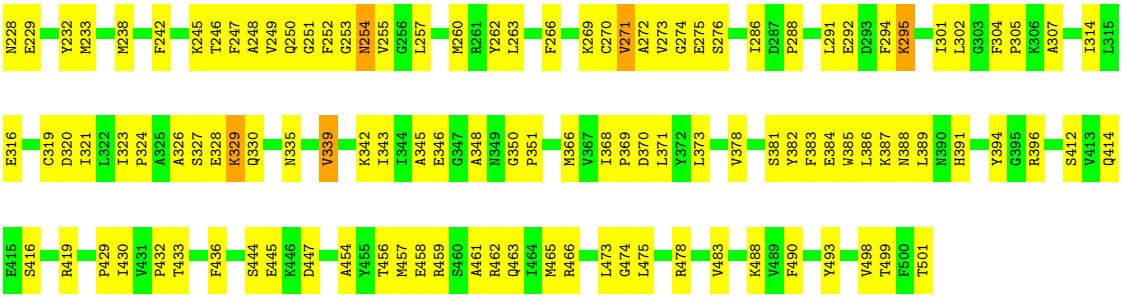
Chain D:




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

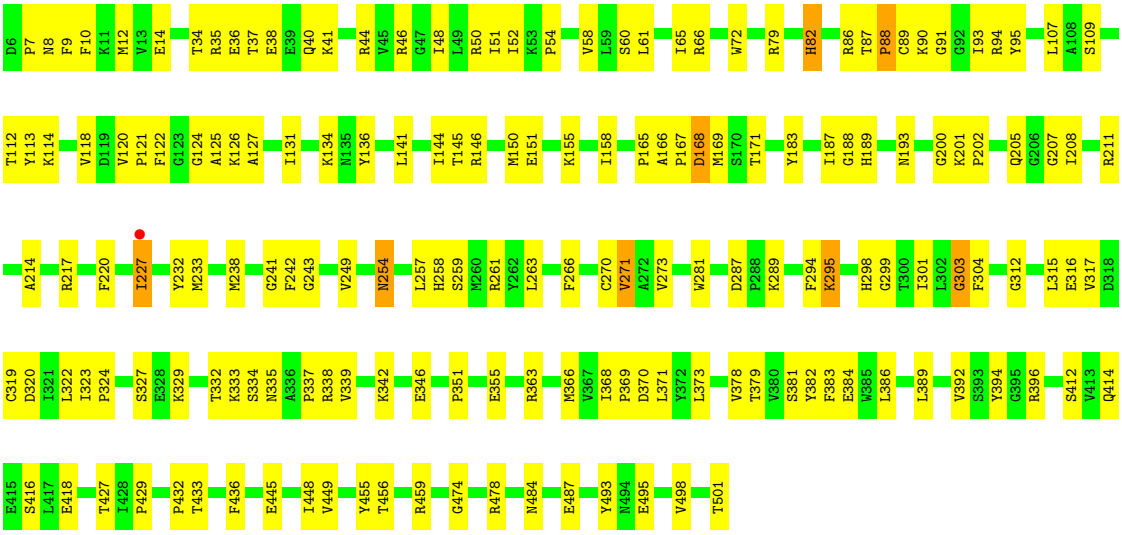
Chain E:





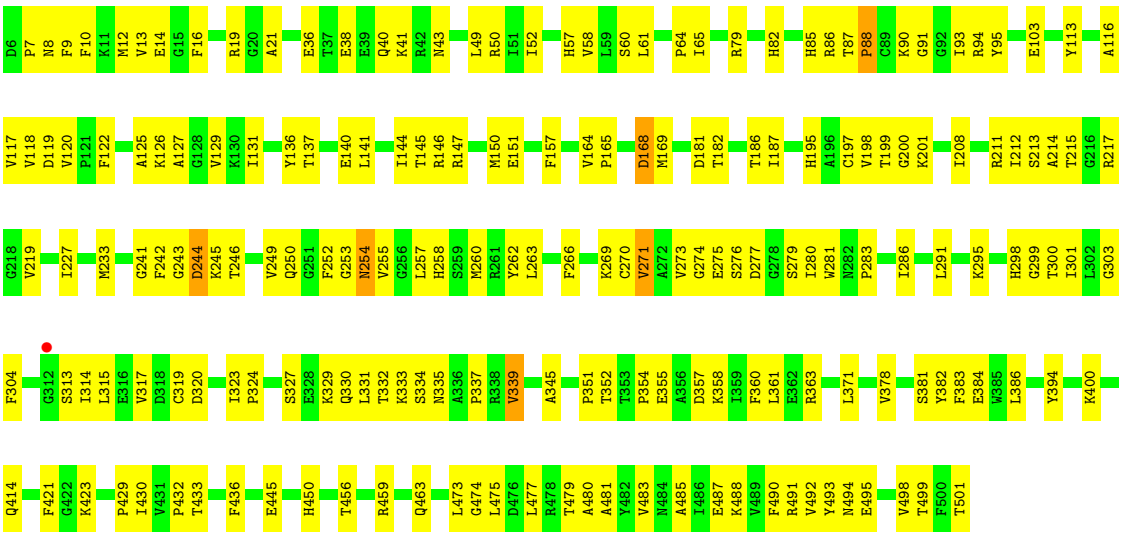
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:



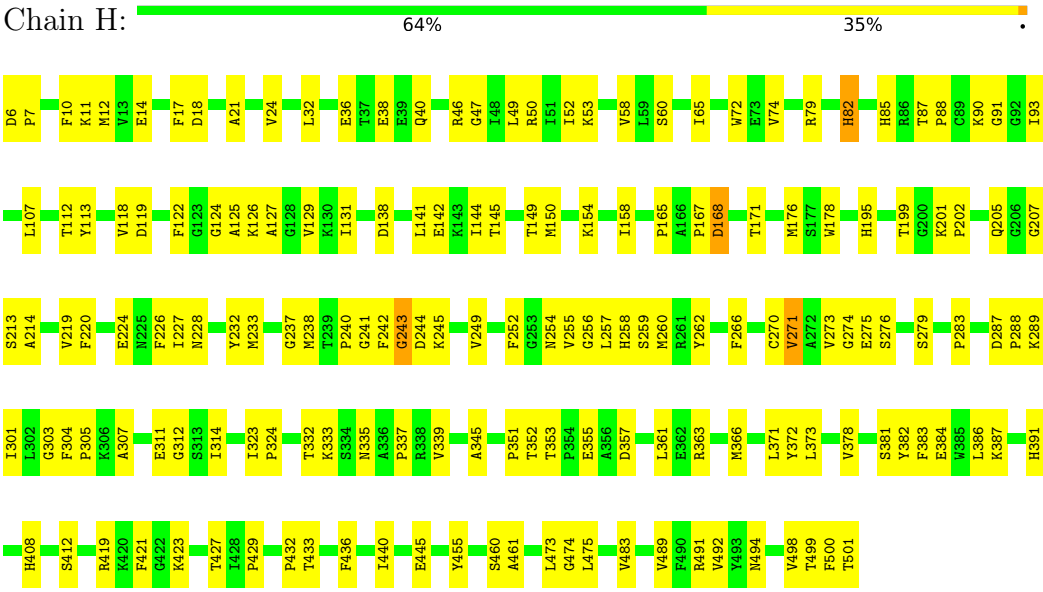
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain G:



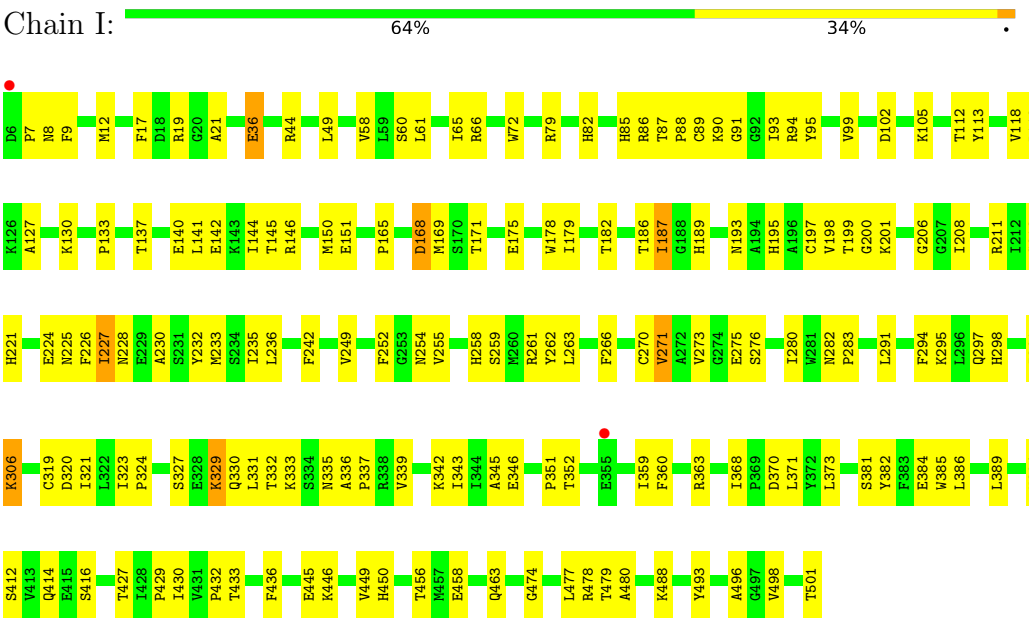
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain H:



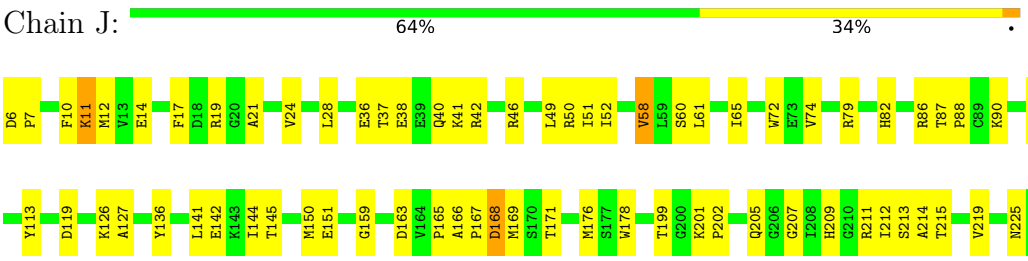

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

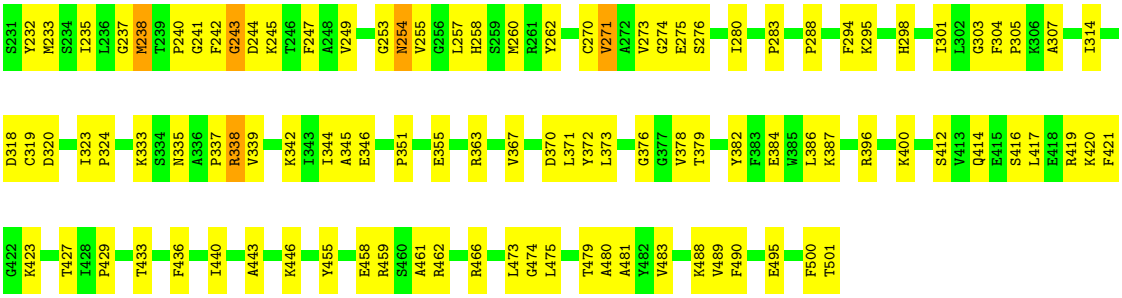
Chain I:




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

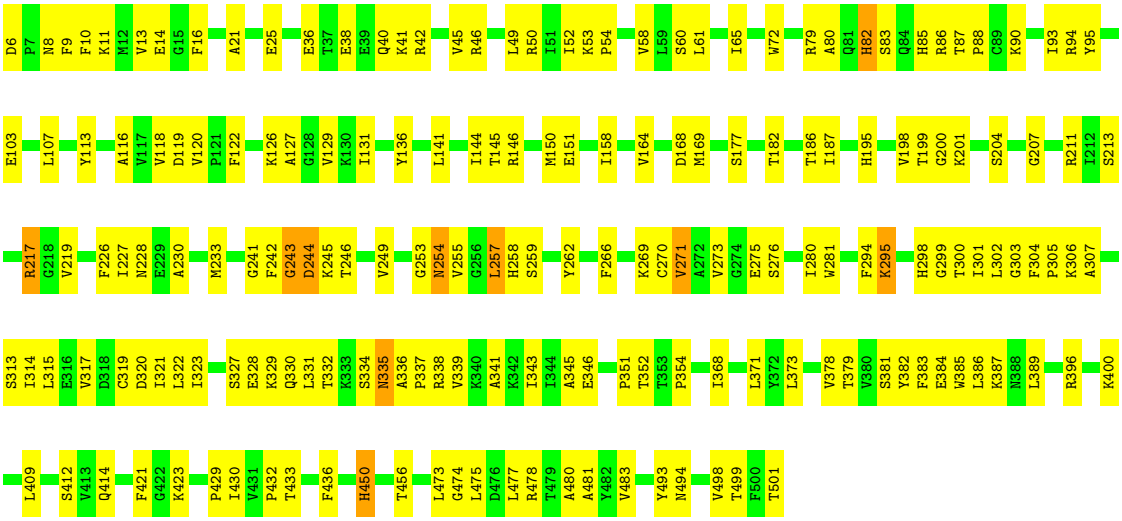
Chain J:





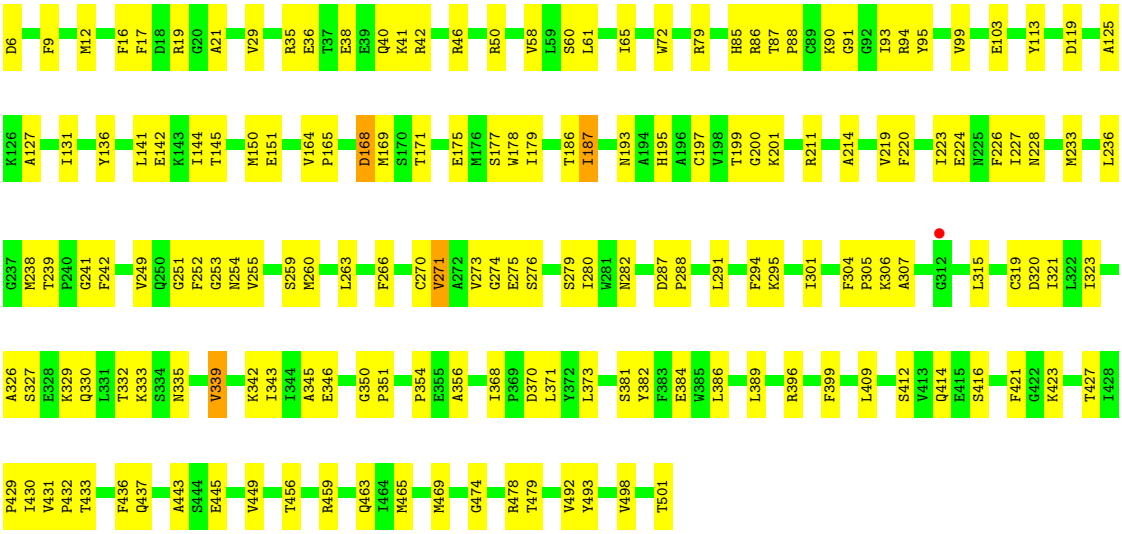
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain K:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain L:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 95.12Å 433.18Å 95.17Å<br>90.00° 118.74° 90.00° | Depositor |
| Resolution (Å) | 49.71 – 3.62<br>49.71 – 3.62 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.5 (49.71-3.62)<br>98.5 (49.71-3.62) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.60 (at 3.67Å) | Xtriage |
| Refinement program | PHENIX (1.12_2829: ???) | Depositor |
| R, $R_{free}$ | 0.246 , 0.314<br>0.249 , 0.314 | Depositor<br>DCC |
| $R_{free}$ test set | 3755 reflections (4.93%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 106.8 | Xtriage |
| Anisotropy | 0.409 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 154.8 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.28$ | Xtriage |
| Estimated twinning fraction | 0.033 for -h-l,k,h<br>0.033 for l,k,-h-l<br>0.038 for h,-k,-h-l<br>0.039 for -h-l,-k,l<br>0.420 for l,-k,h | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 46872 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 129.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: XEG

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 | 0.67 | 6/3957 (0.2%) | 0.78 | 10/5341 (0.2%) |
| 1 | B | 0.17 | 0/3957 | 0.45 | 0/5341 |
| 1 | C | 0.20 | 0/3957 | 0.46 | 2/5341 (0.0%) |
| 1 | D | 0.16 | 0/3957 | 0.45 | 0/5341 |
| 1 | E | 0.16 | 0/3957 | 0.40 | 0/5341 |
| 1 | F | 0.19 | 0/3957 | 0.48 | 2/5341 (0.0%) |
| 1 | G | 0.16 | 0/3957 | 0.42 | 0/5341 |
| 1 | H | 0.17 | 0/3957 | 0.43 | 0/5341 |
| 1 | I | 0.17 | 0/3957 | 0.43 | 2/5341 (0.0%) |
| 1 | J | 0.17 | 0/3957 | 0.41 | 0/5341 |
| 1 | K | 0.23 | 1/3957 (0.0%) | 0.47 | 2/5341 (0.0%) |
| 1 | L | 0.18 | 0/3957 | 0.43 | 0/5341 |
| All | All | 0.26 | 7/47484 (0.0%) | 0.48 | 18/64092 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 2 |
| 1 | C | 0 | 2 |
| 1 | F | 0 | 1 |
| All | All | 0 | 5 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 95 | TYR | CD1-CE1 | 24.77 | 2.12 | 1.38 |
| 1 | A | 95 | TYR | CD2-CE2 | 24.69 | 2.12 | 1.38 |
| 1 | A | 95 | TYR | CG-CD1 | -10.92 | 1.16 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 95 | TYR | CG-CD2 | -10.84 | 1.16 | 1.39 |
| 1 | A | 95 | TYR | CE1-CZ | -10.81 | 1.12 | 1.38 |
| 1 | A | 95 | TYR | CE2-CZ | -10.76 | 1.12 | 1.38 |
| 1 | K | 217 | ARG | CZ-NH2 | -6.98 | 1.24 | 1.33 |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 95 | TYR | CE1-CZ-CE2 | -28.65 | 63.01 | 120.30 |
| 1 | A | 95 | TYR | CD1-CG-CD2 | -23.08 | 83.48 | 118.10 |
| 1 | A | 95 | TYR | CG-CD2-CE2 | -15.49 | 97.97 | 121.20 |
| 1 | A | 95 | TYR | CG-CD1-CE1 | -15.30 | 98.25 | 121.20 |
| 1 | A | 95 | TYR | CB-CG-CD2 | 10.08 | 135.92 | 120.80 |
| 1 | A | 95 | TYR | CB-CG-CD1 | 9.90 | 135.65 | 120.80 |
| 1 | A | 95 | TYR | CE1-CZ-OH | 9.61 | 148.72 | 119.90 |
| 1 | A | 95 | TYR | OH-CZ-CE2 | 9.45 | 148.24 | 119.90 |
| 1 | C | 303 | GLY | CA-C-N | 8.93 | 143.59 | 121.80 |
| 1 | C | 303 | GLY | C-N-CA | 8.93 | 143.59 | 121.80 |
| 1 | F | 303 | GLY | CA-C-N | 8.84 | 143.37 | 121.80 |
| 1 | F | 303 | GLY | C-N-CA | 8.84 | 143.37 | 121.80 |
| 1 | A | 95 | TYR | CD1-CE1-CZ | -6.12 | 108.58 | 119.60 |
| 1 | A | 95 | TYR | CZ-CE2-CD2 | -5.92 | 108.95 | 119.60 |
| 1 | K | 450 | HIS | N-CA-C | -5.75 | 104.98 | 112.23 |
| 1 | I | 303 | GLY | CA-C-N | 5.09 | 134.23 | 121.80 |
| 1 | I | 303 | GLY | C-N-CA | 5.09 | 134.23 | 121.80 |
| 1 | K | 217 | ARG | N-CA-C | -5.02 | 106.67 | 112.89 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 38 | GLU | Peptide |
| 1 | A | 95 | TYR | Sidechain |
| 1 | C | 38 | GLU | Peptide |
| 1 | C | 8 | ASN | Peptide |
| 1 | F | 312 | GLY | Peptide |

## 5.2 Too-close contacts (i)

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 | 3874 | 0 | 3845 | 140 | 0 |
| 1 | B | 3874 | 0 | 3845 | 133 | 0 |
| 1 | C | 3874 | 0 | 3845 | 133 | 0 |
| 1 | D | 3874 | 0 | 3845 | 134 | 0 |
| 1 | E | 3874 | 0 | 3845 | 159 | 0 |
| 1 | F | 3874 | 0 | 3845 | 141 | 0 |
| 1 | G | 3874 | 0 | 3845 | 151 | 0 |
| 1 | H | 3874 | 0 | 3845 | 134 | 0 |
| 1 | I | 3874 | 0 | 3845 | 139 | 0 |
| 1 | J | 3874 | 0 | 3845 | 142 | 0 |
| 1 | K | 3874 | 0 | 3843 | 145 | 0 |
| 1 | L | 3874 | 0 | 3845 | 136 | 0 |
| 2 | A | 32 | 0 | 18 | 1 | 0 |
| 2 | B | 32 | 0 | 18 | 1 | 0 |
| 2 | C | 32 | 0 | 18 | 4 | 0 |
| 2 | D | 32 | 0 | 18 | 2 | 0 |
| 2 | E | 32 | 0 | 18 | 3 | 0 |
| 2 | F | 32 | 0 | 18 | 4 | 0 |
| 2 | G | 32 | 0 | 18 | 4 | 0 |
| 2 | H | 32 | 0 | 18 | 2 | 0 |
| 2 | I | 32 | 0 | 18 | 3 | 0 |
| 2 | J | 32 | 0 | 18 | 6 | 0 |
| 2 | K | 32 | 0 | 18 | 3 | 0 |
| 2 | L | 32 | 0 | 18 | 3 | 0 |
| All | All | 46872 | 0 | 46354 | 1587 | 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 17.

All (1587) 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:E:245:LYS:HE3 | 1:E:320:ASP:CG | 1.70 | 1.15 |
| 1:D:249:VAL:HG12 | 1:D:323:ILE:HD11 | 1.24 | 1.12 |
| 1:C:366:MET:HE1 | 1:C:477:LEU:HD11 | 1.42 | 1.01 |
| 1:E:245:LYS:HE3 | 1:E:320:ASP:OD2 | 1.61 | 1.01 |
| 1:E:238:MET:HE2 | 1:E:245:LYS:HE2 | 1.43 | 1.00 |
| 1:C:366:MET:HE2 | 1:C:475:LEU:HD23 | 1.46 | 0.98 |
| 1:F:249:VAL:HG12 | 1:F:323:ILE:HD11 | 1.45 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:87:THR:HG23 | 1:F:88:PRO:HD3 | 1.45 | 0.97 |
| 1:L:282:ASN:HD21 | 1:L:306:LYS:HG3 | 1.32 | 0.94 |
| 1:E:245:LYS:CE | 1:E:320:ASP:OD2 | 2.16 | 0.93 |
| 1:E:87:THR:HG23 | 1:E:88:PRO:HD3 | 1.50 | 0.93 |
| 1:B:249:VAL:HG12 | 1:B:323:ILE:HD11 | 1.50 | 0.92 |
| 1:J:87:THR:HG23 | 1:J:88:PRO:HD3 | 1.50 | 0.92 |
| 1:L:193:ASN:HD22 | 1:L:389:LEU:HD22 | 1.34 | 0.90 |
| 1:L:282:ASN:ND2 | 1:L:306:LYS:O | 2.04 | 0.90 |
| 1:G:64:PRO:HD2 | 1:G:147:ARG:HH12 | 1.38 | 0.89 |
| 1:A:36:GLU:HG3 | 1:A:38:GLU:HG2 | 1.55 | 0.89 |
| 1:E:245:LYS:NZ | 1:E:320:ASP:OD2 | 2.06 | 0.88 |
| 1:E:304:PHE:HD1 | 1:E:305:PRO:HD2 | 1.40 | 0.87 |
| 1:B:93:ILE:HG22 | 1:B:127:ALA:HB3 | 1.55 | 0.86 |
| 1:C:158:ILE:HD12 | 1:C:165:PRO:HD3 | 1.58 | 0.86 |
| 1:A:249:VAL:HG22 | 1:A:273:VAL:HG22 | 1.58 | 0.86 |
| 1:I:85:HIS:HB3 | 1:I:493:TYR:HE1 | 1.41 | 0.86 |
| 1:K:249:VAL:HG12 | 1:K:323:ILE:HD11 | 1.58 | 0.83 |
| 1:F:169:MET:HE1 | 1:F:327:SER:HA | 1.60 | 0.83 |
| 1:G:87:THR:HG23 | 1:G:88:PRO:HD3 | 1.60 | 0.83 |
| 1:D:249:VAL:HG12 | 1:D:323:ILE:CD1 | 2.06 | 0.82 |
| 1:G:275:GLU:HG2 | 1:G:276:SER:H | 1.44 | 0.82 |
| 1:C:150:MET:HG3 | 1:F:501:THR:HB | 1.62 | 0.82 |
| 1:L:249:VAL:HG12 | 1:L:323:ILE:HD11 | 1.61 | 0.82 |
| 1:F:249:VAL:HG12 | 1:F:323:ILE:CD1 | 2.10 | 0.82 |
| 1:K:254:ASN:H | 1:K:257:LEU:HD12 | 1.45 | 0.81 |
| 1:A:249:VAL:HG12 | 1:A:323:ILE:HD11 | 1.60 | 0.81 |
| 1:L:193:ASN:HD22 | 1:L:389:LEU:CD2 | 1.92 | 0.81 |
| 1:D:193:ASN:HD22 | 1:D:389:LEU:HD22 | 1.43 | 0.81 |
| 1:I:282:ASN:ND2 | 1:I:306:LYS:O | 2.14 | 0.81 |
| 1:B:294:PHE:CD1 | 1:B:298:HIS:HE1 | 1.99 | 0.81 |
| 1:E:245:LYS:CE | 1:E:320:ASP:CG | 2.53 | 0.81 |
| 1:D:93:ILE:HG22 | 1:D:127:ALA:HB3 | 1.63 | 0.80 |
| 1:E:245:LYS:HE3 | 1:E:320:ASP:CB | 2.12 | 0.80 |
| 1:G:212:ILE:HG13 | 1:G:258:HIS:HE1 | 1.46 | 0.80 |
| 1:J:87:THR:CG2 | 1:J:88:PRO:HD3 | 2.11 | 0.79 |
| 1:D:249:VAL:CG1 | 1:D:323:ILE:HD11 | 2.09 | 0.79 |
| 1:E:213:SER:HB3 | 1:E:262:TYR:HE2 | 1.48 | 0.79 |
| 1:K:93:ILE:HG22 | 1:K:127:ALA:HB3 | 1.66 | 0.78 |
| 1:E:93:ILE:HG22 | 1:E:127:ALA:HB3 | 1.64 | 0.78 |
| 1:I:85:HIS:HB3 | 1:I:493:TYR:CE1 | 2.17 | 0.78 |
| 1:K:257:LEU:HD11 | 1:K:295:LYS:HE3 | 1.66 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:93:ILE:HG22 | 1:A:127:ALA:HB3 | 1.63 | 0.78 |
| 1:I:150:MET:HG3 | 1:L:501:THR:HB | 1.65 | 0.78 |
| 1:I:330:GLN:O | 1:I:335:ASN:ND2 | 2.17 | 0.78 |
| 1:C:249:VAL:HG12 | 1:C:323:ILE:HD11 | 1.64 | 0.78 |
| 1:G:249:VAL:HG12 | 1:G:323:ILE:HD11 | 1.66 | 0.77 |
| 1:A:346:GLU:OE1 | 1:A:478:ARG:NH1 | 2.17 | 0.77 |
| 1:C:200:GLY:HA2 | 1:C:211:ARG:HD2 | 1.65 | 0.77 |
| 1:A:219:VAL:HG13 | 1:A:373:LEU:HD21 | 1.66 | 0.77 |
| 1:I:9:PHE:HB3 | 1:I:12:MET:HG2 | 1.66 | 0.77 |
| 1:B:501:THR:HB | 1:E:150:MET:HG3 | 1.66 | 0.77 |
| 1:E:249:VAL:HG12 | 1:E:323:ILE:HD11 | 1.66 | 0.77 |
| 1:G:93:ILE:HG22 | 1:G:127:ALA:HB3 | 1.67 | 0.76 |
| 1:L:93:ILE:HG22 | 1:L:127:ALA:HB3 | 1.67 | 0.76 |
| 1:G:501:THR:HB | 1:J:150:MET:HG3 | 1.67 | 0.76 |
| 1:B:227:ILE:HA | 1:B:233:MET:HE3 | 1.68 | 0.76 |
| 1:H:150:MET:HG3 | 1:K:501:THR:HB | 1.66 | 0.76 |
| 1:A:11:LYS:HG3 | 1:A:14:GLU:HB2 | 1.68 | 0.76 |
| 1:I:319:CYS:SG | 1:I:320:ASP:N | 2.59 | 0.76 |
| 1:J:427:THR:HG22 | 1:J:429:PRO:HD3 | 1.68 | 0.76 |
| 1:C:93:ILE:HG22 | 1:C:127:ALA:HB3 | 1.68 | 0.76 |
| 1:B:275:GLU:O | 1:B:277:ASP:N | 2.19 | 0.75 |
| 1:K:38:GLU:HB2 | 1:K:40:GLN:H | 1.50 | 0.75 |
| 1:D:260:MET:HE3 | 1:D:288:PRO:HB3 | 1.68 | 0.75 |
| 1:F:158:ILE:HD12 | 1:F:165:PRO:HD3 | 1.67 | 0.75 |
| 1:C:38:GLU:HB2 | 1:C:40:GLN:H | 1.51 | 0.75 |
| 1:F:211:ARG:HA | 1:F:214:ALA:HB2 | 1.66 | 0.75 |
| 1:I:93:ILE:HG22 | 1:I:127:ALA:HB3 | 1.67 | 0.75 |
| 1:H:93:ILE:HG22 | 1:H:127:ALA:HB3 | 1.69 | 0.75 |
| 1:E:90:LYS:NZ | 1:E:199:THR:OG1 | 2.19 | 0.75 |
| 1:H:201:LYS:O | 1:H:211:ARG:NH2 | 2.20 | 0.75 |
| 1:J:38:GLU:HB2 | 1:J:40:GLN:H | 1.52 | 0.75 |
| 1:E:249:VAL:HG22 | 1:E:273:VAL:HG22 | 1.66 | 0.74 |
| 1:I:61:LEU:HD21 | 1:I:151:GLU:HB3 | 1.68 | 0.74 |
| 1:K:298:HIS:CE1 | 1:K:304:PHE:HZ | 2.04 | 0.74 |
| 1:J:17:PHE:O | 1:J:21:ALA:N | 2.17 | 0.74 |
| 1:J:93:ILE:HG22 | 1:J:127:ALA:HB3 | 1.69 | 0.74 |
| 1:G:113:TYR:HB2 | 1:G:371:LEU:HD11 | 1.68 | 0.74 |
| 1:A:254:ASN:N | 1:A:257:LEU:HD12 | 2.02 | 0.74 |
| 1:G:291:LEU:HD21 | 1:G:304:PHE:HB2 | 1.69 | 0.74 |
| 1:K:298:HIS:HE1 | 1:K:304:PHE:HZ | 1.34 | 0.74 |
| 1:I:249:VAL:HG12 | 1:I:323:ILE:HD11 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:249:VAL:HG12 | 1:J:323:ILE:HD11 | 1.70 | 0.73 |
| 1:B:294:PHE:HD1 | 1:B:298:HIS:HE1 | 1.35 | 0.73 |
| 1:K:319:CYS:SG | 1:K:320:ASP:N | 2.62 | 0.73 |
| 1:A:36:GLU:HG3 | 1:A:38:GLU:CG | 2.19 | 0.73 |
| 1:D:8:ASN:O | 1:D:9:PHE:HD1 | 1.71 | 0.73 |
| 1:L:327:SER:HB3 | 1:L:330:GLN:HE22 | 1.53 | 0.73 |
| 1:K:200:GLY:HA2 | 1:K:211:ARG:HD2 | 1.70 | 0.73 |
| 1:K:294:PHE:CE2 | 1:K:301:ILE:HA | 2.24 | 0.73 |
| 1:C:427:THR:HG22 | 1:C:429:PRO:HD3 | 1.70 | 0.72 |
| 1:F:61:LEU:HD21 | 1:F:151:GLU:HB3 | 1.71 | 0.72 |
| 1:A:67:ARG:NH2 | 1:A:135:ASN:O | 2.22 | 0.72 |
| 1:K:90:LYS:NZ | 1:K:199:THR:OG1 | 2.22 | 0.72 |
| 1:B:90:LYS:NZ | 1:B:199:THR:OG1 | 2.21 | 0.72 |
| 1:I:498:VAL:HB | 1:L:72:TRP:HH2 | 1.54 | 0.72 |
| 1:B:193:ASN:HD22 | 1:B:389:LEU:HD22 | 1.53 | 0.72 |
| 1:H:427:THR:HG22 | 1:H:429:PRO:HD3 | 1.69 | 0.72 |
| 1:K:327:SER:HB3 | 1:K:330:GLN:HE22 | 1.55 | 0.72 |
| 1:K:332:THR:HG23 | 1:K:334:SER:H | 1.53 | 0.72 |
| 1:H:17:PHE:O | 1:H:21:ALA:N | 2.19 | 0.71 |
| 1:H:287:ASP:OD2 | 1:H:289:LYS:NZ | 2.21 | 0.71 |
| 1:J:319:CYS:SG | 1:J:320:ASP:N | 2.62 | 0.71 |
| 1:A:65:ILE:HD13 | 1:A:144:ILE:HG12 | 1.72 | 0.71 |
| 1:E:219:VAL:HG13 | 1:E:373:LEU:HD21 | 1.70 | 0.71 |
| 1:G:90:LYS:NZ | 1:G:199:THR:OG1 | 2.24 | 0.71 |
| 1:F:242:PHE:HE2 | 1:F:266:PHE:HB3 | 1.56 | 0.71 |
| 1:E:328:GLU:OE1 | 1:E:329:LYS:NZ | 2.23 | 0.71 |
| 1:F:378:VAL:HA | 1:F:381:SER:HB2 | 1.72 | 0.71 |
| 1:G:315:LEU:HD23 | 1:G:315:LEU:H | 1.56 | 0.71 |
| 1:B:327:SER:HB3 | 1:B:330:GLN:HE22 | 1.55 | 0.70 |
| 1:C:249:VAL:HG22 | 1:C:273:VAL:HG22 | 1.74 | 0.70 |
| 1:J:212:ILE:HG13 | 1:J:258:HIS:HE1 | 1.55 | 0.70 |
| 1:H:90:LYS:NZ | 1:H:199:THR:OG1 | 2.24 | 0.70 |
| 1:F:141:LEU:HD12 | 1:F:144:ILE:HD12 | 1.74 | 0.70 |
| 1:J:249:VAL:HG22 | 1:J:273:VAL:HG22 | 1.74 | 0.70 |
| 1:D:271:VAL:HG23 | 1:D:283:PRO:HA | 1.74 | 0.70 |
| 1:F:201:LYS:O | 1:F:211:ARG:NH1 | 2.24 | 0.69 |
| 1:H:58:VAL:HG13 | 1:K:60:SER:HB2 | 1.72 | 0.69 |
| 1:I:219:VAL:HG13 | 1:I:373:LEU:HD21 | 1.72 | 0.69 |
| 1:I:394:TYR:HB2 | 1:I:445:GLU:HG3 | 1.73 | 0.69 |
| 1:A:195:HIS:CE1 | 1:B:87:THR:HG22 | 2.26 | 0.69 |
| 1:A:270:CYS:SG | 1:A:271:VAL:N | 2.64 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:432:PRO:HG2 | 1:L:437:GLN:HG2 | 1.73 | 0.69 |
| 1:A:304:PHE:CD1 | 1:A:305:PRO:HD3 | 2.28 | 0.69 |
| 1:F:168:ASP:N | 1:F:171:THR:OG1 | 2.26 | 0.69 |
| 1:A:56:ASN:HA | 1:D:62:SER:HB3 | 1.74 | 0.69 |
| 1:C:366:MET:CE | 1:C:477:LEU:HD11 | 2.22 | 0.69 |
| 1:G:150:MET:HG3 | 1:J:501:THR:HB | 1.75 | 0.69 |
| 1:K:270:CYS:SG | 1:K:271:VAL:N | 2.66 | 0.68 |
| 1:E:119:ASP:HA | 2:E:601:XEG:HAI | 1.76 | 0.68 |
| 1:C:60:SER:HB2 | 1:F:58:VAL:HG13 | 1.75 | 0.68 |
| 1:L:85:HIS:HB3 | 1:L:493:TYR:HE1 | 1.57 | 0.68 |
| 1:D:87:THR:HG22 | 1:E:195:HIS:CE1 | 2.29 | 0.68 |
| 1:C:262:TYR:HD1 | 1:C:265:ARG:HD2 | 1.59 | 0.68 |
| 1:A:329:LYS:H | 1:A:351:PRO:HA | 1.57 | 0.68 |
| 1:D:319:CYS:SG | 1:D:320:ASP:N | 2.67 | 0.68 |
| 1:F:7:PRO:HD2 | 1:F:329:LYS:HD2 | 1.75 | 0.68 |
| 1:I:72:TRP:HH2 | 1:L:498:VAL:HB | 1.58 | 0.68 |
| 1:J:219:VAL:HG13 | 1:J:373:LEU:HD21 | 1.74 | 0.68 |
| 1:J:459:ARG:NH2 | 2:J:601:XEG:OAH | 2.27 | 0.68 |
| 1:E:246:THR:HG22 | 1:E:269:LYS:HB3 | 1.76 | 0.68 |
| 1:K:280:ILE:HD11 | 1:K:301:ILE:HD11 | 1.76 | 0.68 |
| 1:K:294:PHE:CE1 | 1:K:304:PHE:CE1 | 2.82 | 0.68 |
| 1:F:90:LYS:HD3 | 1:F:378:VAL:HG23 | 1.75 | 0.67 |
| 1:E:304:PHE:CD1 | 1:E:305:PRO:HD2 | 2.26 | 0.67 |
| 1:H:212:ILE:HG13 | 1:H:258:HIS:HE1 | 1.57 | 0.67 |
| 1:K:249:VAL:HG22 | 1:K:273:VAL:HG22 | 1.75 | 0.67 |
| 1:D:90:LYS:NZ | 1:D:199:THR:OG1 | 2.27 | 0.67 |
| 1:J:202:PRO:HG2 | 1:J:205:GLN:HG3 | 1.75 | 0.67 |
| 1:H:219:VAL:HG13 | 1:H:373:LEU:HD21 | 1.76 | 0.67 |
| 1:I:414:GLN:OE1 | 1:I:430:ILE:HG12 | 1.94 | 0.67 |
| 1:E:65:ILE:HD13 | 1:E:144:ILE:HG12 | 1.75 | 0.67 |
| 1:E:238:MET:HE2 | 1:E:245:LYS:CE | 2.23 | 0.67 |
| 1:H:500:PHE:HB3 | 1:J:500:PHE:HB3 | 1.76 | 0.67 |
| 1:H:275:GLU:HG2 | 1:H:276:SER:H | 1.59 | 0.67 |
| 1:H:207:GLY:O | 1:H:387:LYS:NZ | 2.22 | 0.67 |
| 1:I:19:ARG:NE | 1:I:479:THR:HG21 | 2.09 | 0.66 |
| 1:I:280:ILE:HD11 | 1:I:301:ILE:HD11 | 1.77 | 0.66 |
| 1:I:396:ARG:NH1 | 1:K:456:THR:OG1 | 2.28 | 0.66 |
| 1:B:315:LEU:H | 1:B:315:LEU:HD23 | 1.60 | 0.66 |
| 1:L:169:MET:HE1 | 1:L:327:SER:HA | 1.78 | 0.66 |
| 1:A:36:GLU:OE1 | 1:A:44:ARG:NH2 | 2.27 | 0.66 |
| 1:J:119:ASP:HA | 2:J:601:XEG:HAI | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:94:ARG:HG3 | 1:F:169:MET:HB2 | 1.77 | 0.66 |
| 1:K:275:GLU:HG2 | 1:K:276:SER:H | 1.59 | 0.66 |
| 1:B:29:VAL:HB | 1:B:41:LYS:HE3 | 1.77 | 0.66 |
| 1:H:213:SER:HB3 | 1:H:262:TYR:HE2 | 1.60 | 0.66 |
| 1:K:383:PHE:HA | 1:K:386:LEU:HD12 | 1.78 | 0.66 |
| 1:L:427:THR:HG22 | 1:L:429:PRO:HD3 | 1.78 | 0.66 |
| 1:C:181:ASP:OD1 | 1:E:499:THR:OG1 | 2.12 | 0.66 |
| 1:F:79:ARG:HH11 | 1:F:127:ALA:HB2 | 1.61 | 0.66 |
| 1:F:294:PHE:CD2 | 1:F:301:ILE:HD12 | 2.30 | 0.66 |
| 1:K:65:ILE:HD13 | 1:K:144:ILE:HG12 | 1.77 | 0.66 |
| 1:L:90:LYS:NZ | 1:L:199:THR:OG1 | 2.29 | 0.66 |
| 1:A:501:THR:HB | 1:D:150:MET:HG3 | 1.77 | 0.66 |
| 1:B:150:MET:HG3 | 1:E:501:THR:HB | 1.76 | 0.66 |
| 1:K:113:TYR:HB2 | 1:K:371:LEU:HD11 | 1.78 | 0.66 |
| 1:D:323:ILE:HG22 | 1:D:345:ALA:HB3 | 1.76 | 0.66 |
| 1:H:294:PHE:CD2 | 1:H:301:ILE:HD12 | 2.31 | 0.66 |
| 1:B:271:VAL:HG23 | 1:B:283:PRO:HA | 1.76 | 0.66 |
| 1:B:383:PHE:HA | 1:B:386:LEU:HD12 | 1.78 | 0.66 |
| 1:J:337:PRO:O | 1:J:363:ARG:NH2 | 2.29 | 0.65 |
| 1:B:72:TRP:CH2 | 1:E:498:VAL:HB | 2.32 | 0.65 |
| 1:H:304:PHE:H | 1:H:307:ALA:HB3 | 1.59 | 0.65 |
| 1:I:90:LYS:NZ | 1:I:199:THR:OG1 | 2.30 | 0.65 |
| 1:J:275:GLU:HG2 | 1:J:276:SER:H | 1.60 | 0.65 |
| 1:L:249:VAL:HG22 | 1:L:273:VAL:HG22 | 1.77 | 0.65 |
| 1:A:254:ASN:H | 1:A:257:LEU:HD12 | 1.62 | 0.65 |
| 1:C:8:ASN:ND2 | 1:C:355:GLU:OE1 | 2.30 | 0.65 |
| 1:C:58:VAL:HG13 | 1:F:60:SER:HB2 | 1.78 | 0.65 |
| 1:C:113:TYR:HB2 | 1:C:371:LEU:HD11 | 1.79 | 0.65 |
| 1:E:238:MET:HE3 | 1:E:342:LYS:HB2 | 1.77 | 0.65 |
| 1:E:291:LEU:HD11 | 1:E:307:ALA:HB2 | 1.77 | 0.65 |
| 1:I:8:ASN:O | 1:I:329:LYS:NZ | 2.27 | 0.65 |
| 1:L:319:CYS:SG | 1:L:320:ASP:N | 2.69 | 0.65 |
| 1:E:196:ALA:HB2 | 1:E:388:ASN:HB2 | 1.79 | 0.65 |
| 1:F:90:LYS:NZ | 1:F:381:SER:HB3 | 2.12 | 0.65 |
| 1:E:61:LEU:HD21 | 1:E:151:GLU:HB3 | 1.79 | 0.64 |
| 1:I:211:ARG:HA | 1:I:214:ALA:HB2 | 1.78 | 0.64 |
| 1:E:291:LEU:HD21 | 1:E:304:PHE:HB2 | 1.78 | 0.64 |
| 1:C:24:VAL:HG12 | 1:C:28:LEU:HG | 1.78 | 0.64 |
| 1:B:61:LEU:HD21 | 1:B:151:GLU:HB3 | 1.80 | 0.64 |
| 1:I:498:VAL:HB | 1:L:72:TRP:CH2 | 2.32 | 0.64 |
| 1:L:113:TYR:HB2 | 1:L:371:LEU:HD11 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:227:ILE:HA | 1:D:233:MET:HE3 | 1.78 | 0.64 |
| 1:F:249:VAL:HG22 | 1:F:273:VAL:HG22 | 1.80 | 0.64 |
| 1:F:258:HIS:HA | 1:F:261:ARG:HB3 | 1.80 | 0.64 |
| 1:L:9:PHE:CZ | 1:L:354:PRO:HD2 | 2.33 | 0.64 |
| 1:A:90:LYS:NZ | 1:A:199:THR:OG1 | 2.29 | 0.64 |
| 1:B:168:ASP:N | 1:B:171:THR:OG1 | 2.31 | 0.64 |
| 1:B:323:ILE:HG22 | 1:B:345:ALA:HB3 | 1.78 | 0.64 |
| 1:J:323:ILE:HG22 | 1:J:345:ALA:HB3 | 1.80 | 0.64 |
| 1:I:456:THR:OG1 | 1:J:396:ARG:NH1 | 2.29 | 0.64 |
| 1:J:274:GLY:HA3 | 1:J:314:ILE:HD13 | 1.80 | 0.64 |
| 1:F:394:TYR:HB3 | 1:F:448:ILE:HD12 | 1.80 | 0.64 |
| 1:K:315:LEU:HD22 | 1:K:322:LEU:HD21 | 1.78 | 0.63 |
| 1:C:456:THR:OG1 | 1:D:396:ARG:NH1 | 2.32 | 0.63 |
| 1:I:275:GLU:HG2 | 1:I:276:SER:H | 1.63 | 0.63 |
| 1:I:427:THR:HG22 | 1:I:429:PRO:HD3 | 1.81 | 0.63 |
| 1:J:61:LEU:HD21 | 1:J:151:GLU:HB3 | 1.80 | 0.63 |
| 1:J:207:GLY:O | 1:J:387:LYS:NZ | 2.25 | 0.63 |
| 1:E:328:GLU:HG2 | 1:E:329:LYS:HG3 | 1.81 | 0.63 |
| 1:H:412:SER:HB3 | 1:L:432:PRO:HA | 1.81 | 0.63 |
| 1:L:193:ASN:ND2 | 1:L:389:LEU:HD22 | 2.10 | 0.63 |
| 1:G:60:SER:HB2 | 1:J:58:VAL:HG13 | 1.80 | 0.63 |
| 1:J:168:ASP:N | 1:J:171:THR:OG1 | 2.29 | 0.63 |
| 1:B:126:LYS:NZ | 1:B:168:ASP:OD2 | 2.29 | 0.63 |
| 1:B:204:SER:OG | 1:F:495:GLU:OE1 | 2.17 | 0.63 |
| 1:G:65:ILE:HD13 | 1:G:144:ILE:HG12 | 1.79 | 0.63 |
| 1:K:79:ARG:HH11 | 1:K:127:ALA:HB2 | 1.63 | 0.63 |
| 1:A:113:TYR:HB2 | 1:A:371:LEU:HD11 | 1.79 | 0.63 |
| 1:B:11:LYS:HB2 | 1:B:14:GLU:HB2 | 1.80 | 0.63 |
| 1:D:11:LYS:HB2 | 1:D:14:GLU:HB2 | 1.81 | 0.63 |
| 1:F:79:ARG:HD2 | 1:F:127:ALA:HB2 | 1.79 | 0.63 |
| 1:F:211:ARG:NE | 1:F:384:GLU:OE2 | 2.32 | 0.63 |
| 1:A:499:THR:HG22 | 1:A:501:THR:HG23 | 1.80 | 0.63 |
| 1:C:107:LEU:HD23 | 1:C:126:LYS:HE2 | 1.80 | 0.63 |
| 1:E:245:LYS:HE3 | 1:E:320:ASP:HB3 | 1.80 | 0.63 |
| 1:F:158:ILE:HD12 | 1:F:165:PRO:CD | 2.29 | 0.63 |
| 1:G:249:VAL:HG22 | 1:G:273:VAL:HG22 | 1.81 | 0.62 |
| 1:G:319:CYS:SG | 1:G:320:ASP:N | 2.72 | 0.62 |
| 1:A:150:MET:HG3 | 1:D:501:THR:HB | 1.81 | 0.62 |
| 1:A:383:PHE:HA | 1:A:386:LEU:HD12 | 1.81 | 0.62 |
| 1:J:107:LEU:HD23 | 1:J:126:LYS:HE2 | 1.81 | 0.62 |
| 1:L:85:HIS:HB3 | 1:L:493:TYR:CE1 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:315:LEU:HD23 | 1:L:315:LEU:H | 1.64 | 0.62 |
| 1:L:294:PHE:CE2 | 1:L:301:ILE:HA | 2.34 | 0.62 |
| 1:I:94:ARG:HG3 | 1:I:169:MET:HB2 | 1.81 | 0.62 |
| 1:L:19:ARG:NE | 1:L:479:THR:HG21 | 2.15 | 0.62 |
| 1:D:378:VAL:O | 1:D:382:TYR:N | 2.32 | 0.62 |
| 1:I:19:ARG:HE | 1:I:479:THR:HG21 | 1.64 | 0.62 |
| 1:J:294:PHE:CE2 | 1:J:301:ILE:HG13 | 2.33 | 0.62 |
| 1:L:275:GLU:HG2 | 1:L:276:SER:H | 1.64 | 0.62 |
| 1:D:93:ILE:HD11 | 1:D:176:MET:HE1 | 1.81 | 0.62 |
| 1:E:346:GLU:OE1 | 1:E:478:ARG:NH1 | 2.32 | 0.62 |
| 1:G:327:SER:HB3 | 1:G:330:GLN:HE22 | 1.63 | 0.62 |
| 1:H:337:PRO:O | 1:H:363:ARG:NH2 | 2.32 | 0.62 |
| 1:E:48:ILE:O | 1:E:52:ILE:HG13 | 2.00 | 0.62 |
| 1:L:38:GLU:HB2 | 1:L:40:GLN:H | 1.64 | 0.62 |
| 1:G:227:ILE:HG23 | 1:G:233:MET:HE3 | 1.81 | 0.62 |
| 1:J:24:VAL:HG13 | 1:J:483:VAL:HG23 | 1.82 | 0.62 |
| 1:A:58:VAL:HG13 | 1:D:60:SER:OG | 2.00 | 0.62 |
| 1:A:433:THR:HG23 | 1:A:436:PHE:H | 1.64 | 0.62 |
| 1:E:29:VAL:HB | 1:E:41:LYS:HD3 | 1.81 | 0.62 |
| 1:E:304:PHE:H | 1:E:307:ALA:HB3 | 1.65 | 0.62 |
| 1:F:200:GLY:HA2 | 1:F:211:ARG:HD2 | 1.82 | 0.62 |
| 1:G:300:THR:HG22 | 1:G:301:ILE:N | 2.15 | 0.62 |
| 1:A:498:VAL:HB | 1:D:72:TRP:CH2 | 2.35 | 0.61 |
| 1:G:400:LYS:HB2 | 1:H:455:TYR:HB2 | 1.81 | 0.61 |
| 1:H:240:PRO:O | 1:H:242:PHE:N | 2.32 | 0.61 |
| 1:H:501:THR:HB | 1:K:150:MET:HG3 | 1.80 | 0.61 |
| 1:G:201:LYS:O | 1:G:211:ARG:NH2 | 2.33 | 0.61 |
| 1:D:249:VAL:CG2 | 1:D:273:VAL:HG22 | 2.29 | 0.61 |
| 1:E:250:GLN:HE22 | 1:E:330:GLN:HE21 | 1.47 | 0.61 |
| 1:G:456:THR:OG1 | 1:L:396:ARG:NH1 | 2.28 | 0.61 |
| 1:J:213:SER:HB3 | 1:J:262:TYR:HE2 | 1.64 | 0.61 |
| 1:J:480:ALA:HA | 1:J:483:VAL:CG1 | 2.29 | 0.61 |
| 1:F:227:ILE:HG23 | 1:F:233:MET:HE3 | 1.82 | 0.61 |
| 1:H:396:ARG:NH2 | 1:L:119:ASP:O | 2.33 | 0.61 |
| 1:K:298:HIS:HE1 | 1:K:304:PHE:CZ | 2.18 | 0.61 |
| 1:A:81:GLN:NE2 | 1:A:163:ASP:OD1 | 2.33 | 0.61 |
| 1:C:303:GLY:O | 1:C:304:PHE:HD1 | 1.83 | 0.61 |
| 1:G:94:ARG:HG3 | 1:G:169:MET:HB2 | 1.83 | 0.61 |
| 1:G:181:ASP:OD1 | 1:H:499:THR:OG1 | 2.19 | 0.61 |
| 1:B:79:ARG:HH11 | 1:B:127:ALA:HB2 | 1.64 | 0.61 |
| 1:C:57:HIS:CD2 | 1:F:155:LYS:HE3 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:17:PHE:O | 1:I:21:ALA:N | 2.32 | 0.61 |
| 1:I:433:THR:HG23 | 1:I:436:PHE:H | 1.65 | 0.61 |
| 1:C:378:VAL:HA | 1:C:381:SER:HB2 | 1.82 | 0.61 |
| 1:E:81:GLN:NE2 | 1:E:163:ASP:OD1 | 2.33 | 0.61 |
| 1:F:319:CYS:SG | 1:F:320:ASP:N | 2.74 | 0.61 |
| 1:G:270:CYS:SG | 1:G:271:VAL:N | 2.73 | 0.61 |
| 1:H:323:ILE:HG22 | 1:H:345:ALA:HB3 | 1.83 | 0.61 |
| 1:J:119:ASP:O | 1:K:396:ARG:NH2 | 2.30 | 0.61 |
| 1:A:48:ILE:O | 1:A:52:ILE:HG13 | 2.00 | 0.61 |
| 1:F:90:LYS:HZ2 | 1:F:381:SER:HB3 | 1.66 | 0.61 |
| 1:F:298:HIS:CE1 | 1:F:304:PHE:HZ | 2.19 | 0.61 |
| 1:H:87:THR:OG1 | 1:H:88:PRO:HD3 | 2.01 | 0.61 |
| 1:H:421:PHE:CZ | 1:H:423:LYS:HB2 | 2.36 | 0.61 |
| 1:L:433:THR:HG23 | 1:L:436:PHE:H | 1.65 | 0.61 |
| 1:A:432:PRO:HA | 1:F:412:SER:HB3 | 1.81 | 0.60 |
| 1:C:79:ARG:HH11 | 1:C:127:ALA:HB2 | 1.66 | 0.60 |
| 1:L:219:VAL:HG13 | 1:L:373:LEU:HD21 | 1.83 | 0.60 |
| 1:C:394:TYR:HB2 | 1:C:445:GLU:HG3 | 1.82 | 0.60 |
| 1:D:36:GLU:OE1 | 1:D:41:LYS:HG2 | 2.02 | 0.60 |
| 1:F:113:TYR:HB2 | 1:F:371:LEU:HD11 | 1.82 | 0.60 |
| 1:G:303:GLY:O | 1:G:304:PHE:HD1 | 1.83 | 0.60 |
| 1:F:427:THR:HG22 | 1:F:429:PRO:HD3 | 1.83 | 0.60 |
| 1:E:87:THR:CG2 | 1:E:88:PRO:HD3 | 2.27 | 0.60 |
| 1:I:169:MET:HE1 | 1:I:327:SER:HA | 1.84 | 0.60 |
| 1:K:131:ILE:HB | 1:K:136:TYR:CE2 | 2.37 | 0.60 |
| 1:A:196:ALA:HB2 | 1:A:388:ASN:HB2 | 1.82 | 0.60 |
| 1:I:294:PHE:CE2 | 1:I:301:ILE:HA | 2.35 | 0.60 |
| 1:J:225:ASN:ND2 | 1:J:458:GLU:HA | 2.17 | 0.60 |
| 1:F:87:THR:CG2 | 1:F:88:PRO:HD3 | 2.26 | 0.60 |
| 1:H:274:GLY:HA3 | 1:H:314:ILE:HD13 | 1.82 | 0.60 |
| 1:E:67:ARG:NH2 | 1:E:135:ASN:O | 2.35 | 0.60 |
| 1:H:433:THR:HG23 | 1:H:436:PHE:H | 1.67 | 0.60 |
| 1:I:113:TYR:HB2 | 1:I:371:LEU:HD11 | 1.83 | 0.60 |
| 1:C:72:TRP:HH2 | 1:F:498:VAL:HB | 1.66 | 0.60 |
| 1:H:21:ALA:HB1 | 1:H:49:LEU:HD23 | 1.83 | 0.60 |
| 1:D:168:ASP:N | 1:D:171:THR:OG1 | 2.34 | 0.59 |
| 1:G:38:GLU:HB2 | 1:G:40:GLN:H | 1.66 | 0.59 |
| 1:G:490:PHE:HE2 | 1:G:494:ASN:HD22 | 1.50 | 0.59 |
| 1:J:136:TYR:HB2 | 1:J:141:LEU:CD1 | 2.33 | 0.59 |
| 1:I:249:VAL:HG22 | 1:I:273:VAL:HG22 | 1.83 | 0.59 |
| 1:L:315:LEU:HD12 | 1:L:339:VAL:HG22 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:282:ASN:ND2 | 1:A:306:LYS:O | 2.34 | 0.59 |
| 1:C:72:TRP:CH2 | 1:F:498:VAL:HB | 2.36 | 0.59 |
| 1:D:219:VAL:HG13 | 1:D:373:LEU:HD21 | 1.82 | 0.59 |
| 1:J:79:ARG:HH11 | 1:J:127:ALA:HB2 | 1.67 | 0.59 |
| 1:K:254:ASN:N | 1:K:257:LEU:HD12 | 2.17 | 0.59 |
| 1:B:58:VAL:HG13 | 1:E:60:SER:OG | 2.03 | 0.59 |
| 1:H:249:VAL:HG12 | 1:H:323:ILE:HD11 | 1.83 | 0.59 |
| 1:E:12:MET:HG2 | 1:E:329:LYS:HD3 | 1.84 | 0.59 |
| 1:K:303:GLY:O | 1:K:304:PHE:HD1 | 1.85 | 0.59 |
| 1:G:300:THR:HG22 | 1:G:301:ILE:H | 1.65 | 0.59 |
| 1:J:10:PHE:O | 1:J:12:MET:N | 2.35 | 0.59 |
| 1:G:79:ARG:HD3 | 1:G:157:PHE:HB3 | 1.85 | 0.59 |
| 1:J:240:PRO:O | 1:J:242:PHE:N | 2.36 | 0.59 |
| 1:J:280:ILE:HD11 | 1:J:301:ILE:HD11 | 1.84 | 0.59 |
| 1:G:498:VAL:HB | 1:J:72:TRP:HH2 | 1.68 | 0.59 |
| 1:J:11:LYS:HB2 | 1:J:14:GLU:HB2 | 1.84 | 0.59 |
| 1:K:118:VAL:HG23 | 1:K:120:VAL:HG23 | 1.83 | 0.59 |
| 1:K:249:VAL:HA | 1:K:323:ILE:HG13 | 1.85 | 0.59 |
| 1:D:213:SER:HA | 1:D:258:HIS:ND1 | 2.18 | 0.58 |
| 1:G:323:ILE:HG22 | 1:G:345:ALA:HB3 | 1.85 | 0.58 |
| 1:G:332:THR:HG23 | 1:G:334:SER:H | 1.68 | 0.58 |
| 1:K:6:ASP:HB3 | 1:K:332:THR:HG21 | 1.85 | 0.58 |
| 1:L:142:GLU:HG3 | 1:L:178:TRP:CD2 | 2.38 | 0.58 |
| 1:L:270:CYS:SG | 1:L:271:VAL:N | 2.76 | 0.58 |
| 1:B:304:PHE:H | 1:B:307:ALA:HB3 | 1.68 | 0.58 |
| 1:C:90:LYS:HG3 | 1:C:122:PHE:CD1 | 2.38 | 0.58 |
| 1:C:294:PHE:CD2 | 1:C:301:ILE:HD12 | 2.38 | 0.58 |
| 1:G:211:ARG:HA | 1:G:214:ALA:HB2 | 1.85 | 0.58 |
| 1:J:142:GLU:HG3 | 1:J:178:TRP:CE2 | 2.39 | 0.58 |
| 1:A:456:THR:OG1 | 1:F:396:ARG:NH1 | 2.37 | 0.58 |
| 1:D:249:VAL:HG22 | 1:D:273:VAL:HG22 | 1.86 | 0.58 |
| 1:H:113:TYR:HB2 | 1:H:371:LEU:HD11 | 1.85 | 0.58 |
| 1:L:414:GLN:OE1 | 1:L:430:ILE:HG12 | 2.04 | 0.58 |
| 1:G:58:VAL:HG13 | 1:J:60:SER:HB2 | 1.85 | 0.58 |
| 1:G:429:PRO:HA | 1:L:416:SER:HB3 | 1.85 | 0.58 |
| 1:H:212:ILE:HG13 | 1:H:258:HIS:CE1 | 2.39 | 0.58 |
| 1:I:58:VAL:HG13 | 1:L:60:SER:HB2 | 1.86 | 0.58 |
| 1:G:57:HIS:HE2 | 1:J:151:GLU:HG3 | 1.68 | 0.58 |
| 1:B:94:ARG:NH1 | 1:B:103:GLU:OE2 | 2.37 | 0.58 |
| 1:H:233:MET:O | 1:H:237:GLY:N | 2.36 | 0.58 |
| 1:D:46:ARG:HG2 | 1:D:50:ARG:HH11 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:473:LEU:O | 1:D:475:LEU:N | 2.36 | 0.58 |
| 1:I:208:ILE:HG22 | 1:I:211:ARG:HD3 | 1.86 | 0.58 |
| 1:J:480:ALA:C | 1:J:483:VAL:HG12 | 2.28 | 0.58 |
| 1:L:321:ILE:HA | 1:L:343:ILE:O | 2.04 | 0.58 |
| 1:D:350:GLY:N | 1:D:370:ASP:OD2 | 2.37 | 0.58 |
| 1:I:501:THR:HB | 1:L:150:MET:HG3 | 1.86 | 0.58 |
| 1:J:480:ALA:HA | 1:J:483:VAL:HG12 | 1.84 | 0.58 |
| 1:E:385:TRP:O | 1:E:389:LEU:HG | 2.04 | 0.57 |
| 1:F:270:CYS:SG | 1:F:271:VAL:N | 2.77 | 0.57 |
| 1:F:414:GLN:HB2 | 1:F:429:PRO:HD2 | 1.87 | 0.57 |
| 1:I:72:TRP:CH2 | 1:L:498:VAL:HB | 2.39 | 0.57 |
| 1:L:323:ILE:HG22 | 1:L:345:ALA:HB3 | 1.84 | 0.57 |
| 1:C:141:LEU:HD12 | 1:C:144:ILE:HD12 | 1.87 | 0.57 |
| 1:G:146:ARG:HG2 | 1:G:182:THR:OG1 | 2.04 | 0.57 |
| 1:K:146:ARG:HG2 | 1:K:182:THR:OG1 | 2.04 | 0.57 |
| 1:A:498:VAL:HB | 1:D:72:TRP:HH2 | 1.69 | 0.57 |
| 1:F:394:TYR:HB2 | 1:F:445:GLU:HG3 | 1.86 | 0.57 |
| 1:I:432:PRO:HA | 1:J:412:SER:HB3 | 1.86 | 0.57 |
| 1:J:433:THR:HG23 | 1:J:436:PHE:H | 1.69 | 0.57 |
| 1:K:21:ALA:HB1 | 1:K:49:LEU:HD23 | 1.87 | 0.57 |
| 1:A:87:THR:HB | 1:A:88:PRO:HD3 | 1.87 | 0.57 |
| 1:A:396:ARG:NE | 2:B:601:XEG:OAF | 2.34 | 0.57 |
| 1:G:200:GLY:H | 1:G:384:GLU:CD | 2.13 | 0.57 |
| 1:H:294:PHE:CE2 | 1:H:301:ILE:HA | 2.39 | 0.57 |
| 1:C:400:LYS:NZ | 1:E:458:GLU:OE1 | 2.36 | 0.57 |
| 1:G:79:ARG:HH11 | 1:G:127:ALA:HB2 | 1.69 | 0.57 |
| 1:J:90:LYS:NZ | 1:J:199:THR:OG1 | 2.35 | 0.57 |
| 1:A:12:MET:SD | 1:A:329:LYS:HD2 | 2.44 | 0.57 |
| 1:B:91:GLY:HA3 | 1:B:125:ALA:O | 2.04 | 0.57 |
| 1:B:270:CYS:SG | 1:B:271:VAL:N | 2.77 | 0.57 |
| 1:C:118:VAL:HG23 | 1:C:120:VAL:HG23 | 1.87 | 0.57 |
| 1:D:79:ARG:HH11 | 1:D:127:ALA:HB2 | 1.69 | 0.57 |
| 1:I:291:LEU:CD1 | 1:I:304:PHE:HD2 | 2.17 | 0.57 |
| 1:B:60:SER:OG | 1:E:58:VAL:HG13 | 2.05 | 0.57 |
| 1:D:10:PHE:O | 1:D:12:MET:N | 2.36 | 0.57 |
| 1:G:195:HIS:CD2 | 1:H:87:THR:CG2 | 2.88 | 0.57 |
| 1:G:212:ILE:HG13 | 1:G:258:HIS:CE1 | 2.34 | 0.57 |
| 1:H:72:TRP:HH2 | 1:K:498:VAL:HB | 1.70 | 0.57 |
| 1:A:260:MET:HE1 | 1:A:286:ILE:HD11 | 1.87 | 0.57 |
| 1:E:242:PHE:CE2 | 1:E:266:PHE:HB3 | 2.39 | 0.57 |
| 1:C:258:HIS:HA | 1:C:261:ARG:HB3 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:294:PHE:CD2 | 1:I:301:ILE:HD12 | 2.40 | 0.57 |
| 1:I:323:ILE:HG22 | 1:I:345:ALA:HB3 | 1.87 | 0.57 |
| 1:A:429:PRO:HA | 1:F:416:SER:HB3 | 1.86 | 0.57 |
| 1:B:303:GLY:O | 1:B:304:PHE:HD1 | 1.87 | 0.57 |
| 1:E:29:VAL:HG12 | 1:E:41:LYS:HB2 | 1.87 | 0.57 |
| 1:H:168:ASP:N | 1:H:171:THR:OG1 | 2.37 | 0.57 |
| 1:L:242:PHE:HE2 | 1:L:266:PHE:HB3 | 1.69 | 0.57 |
| 1:I:332:THR:OG1 | 1:I:333:LYS:N | 2.37 | 0.56 |
| 1:F:334:SER:O | 1:F:338:ARG:NH2 | 2.38 | 0.56 |
| 1:G:337:PRO:O | 1:G:363:ARG:NH2 | 2.38 | 0.56 |
| 1:A:168:ASP:H | 1:A:171:THR:HG1 | 1.52 | 0.56 |
| 1:B:65:ILE:HD13 | 1:B:144:ILE:HG12 | 1.85 | 0.56 |
| 1:B:378:VAL:O | 1:B:382:TYR:N | 2.38 | 0.56 |
| 1:C:37:THR:HA | 1:C:41:LYS:HD2 | 1.87 | 0.56 |
| 1:E:254:ASN:H | 1:E:257:LEU:HD12 | 1.70 | 0.56 |
| 1:F:36:GLU:HG3 | 1:F:37:THR:N | 2.20 | 0.56 |
| 1:H:60:SER:HB2 | 1:K:58:VAL:HG13 | 1.88 | 0.56 |
| 1:K:88:PRO:HG2 | 1:K:122:PHE:CE2 | 2.41 | 0.56 |
| 1:L:9:PHE:HZ | 1:L:354:PRO:HD2 | 1.69 | 0.56 |
| 1:L:186:THR:OG1 | 1:L:187:ILE:N | 2.38 | 0.56 |
| 1:L:274:GLY:HA2 | 1:L:279:SER:HA | 1.85 | 0.56 |
| 1:K:323:ILE:HG22 | 1:K:345:ALA:HB3 | 1.87 | 0.56 |
| 1:L:165:PRO:HD2 | 1:L:197:CYS:O | 2.05 | 0.56 |
| 1:A:213:SER:HB3 | 1:A:262:TYR:HE2 | 1.71 | 0.56 |
| 1:A:348:ALA:HB3 | 1:A:351:PRO:HG3 | 1.87 | 0.56 |
| 1:B:151:GLU:HG3 | 1:E:57:HIS:HE2 | 1.71 | 0.56 |
| 1:D:6:ASP:O | 1:D:8:ASN:N | 2.39 | 0.56 |
| 1:B:211:ARG:HA | 1:B:214:ALA:HB2 | 1.88 | 0.56 |
| 1:C:498:VAL:HB | 1:F:72:TRP:CH2 | 2.40 | 0.56 |
| 1:E:13:VAL:HA | 1:E:16:PHE:CD2 | 2.40 | 0.56 |
| 1:G:432:PRO:HA | 1:L:412:SER:HB3 | 1.88 | 0.56 |
| 1:I:85:HIS:CD2 | 1:I:86:ARG:HG2 | 2.41 | 0.56 |
| 1:D:65:ILE:HD13 | 1:D:144:ILE:HG12 | 1.88 | 0.56 |
| 1:D:331:LEU:HA | 1:D:335:ASN:HD21 | 1.70 | 0.56 |
| 1:I:458:GLU:OE1 | 1:J:400:LYS:NZ | 2.37 | 0.56 |
| 1:L:61:LEU:HD21 | 1:L:151:GLU:HB2 | 1.88 | 0.56 |
| 1:L:200:GLY:HA2 | 1:L:211:ARG:HD2 | 1.88 | 0.56 |
| 1:A:60:SER:HB2 | 1:D:58:VAL:CG1 | 2.36 | 0.56 |
| 1:C:181:ASP:O | 1:C:185:SER:OG | 2.18 | 0.56 |
| 1:I:36:GLU:HG3 | 1:I:44:ARG:HH21 | 1.69 | 0.56 |
| 1:K:255:VAL:O | 1:K:259:SER:OG | 2.16 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:329:LYS:H | 1:L:351:PRO:HA | 1.71 | 0.56 |
| 1:A:94:ARG:HE | 1:A:169:MET:HG3 | 1.70 | 0.56 |
| 1:B:408:HIS:O | 1:B:412:SER:OG | 2.20 | 0.56 |
| 1:F:249:VAL:CG2 | 1:F:273:VAL:HG22 | 2.36 | 0.56 |
| 1:I:321:ILE:HA | 1:I:343:ILE:O | 2.05 | 0.56 |
| 1:J:243:GLY:O | 1:J:245:LYS:N | 2.39 | 0.56 |
| 1:C:213:SER:HB3 | 1:C:262:TYR:HE2 | 1.70 | 0.56 |
| 1:C:296:LEU:HD21 | 1:E:35:ARG:HG3 | 1.87 | 0.56 |
| 1:E:113:TYR:HB2 | 1:E:371:LEU:HD11 | 1.87 | 0.56 |
| 1:J:270:CYS:SG | 1:J:271:VAL:N | 2.77 | 0.56 |
| 1:L:94:ARG:HD3 | 1:L:169:MET:HB2 | 1.88 | 0.56 |
| 1:L:94:ARG:NH2 | 1:L:169:MET:SD | 2.79 | 0.56 |
| 1:L:282:ASN:ND2 | 1:L:306:LYS:HG3 | 2.13 | 0.56 |
| 1:C:158:ILE:CD1 | 1:C:165:PRO:HD3 | 2.34 | 0.55 |
| 1:J:382:TYR:CZ | 1:J:386:LEU:HD11 | 2.40 | 0.55 |
| 1:D:421:PHE:CZ | 1:D:423:LYS:HB2 | 2.42 | 0.55 |
| 1:H:141:LEU:HD12 | 1:H:144:ILE:HD12 | 1.88 | 0.55 |
| 1:H:213:SER:HB3 | 1:H:262:TYR:CE2 | 2.41 | 0.55 |
| 1:H:227:ILE:HA | 1:H:233:MET:HE2 | 1.88 | 0.55 |
| 1:K:95:TYR:OH | 1:K:145:THR:HG22 | 2.06 | 0.55 |
| 1:I:165:PRO:HD2 | 1:I:197:CYS:O | 2.07 | 0.55 |
| 1:K:217:ARG:CZ | 1:K:450:HIS:CE1 | 2.78 | 0.55 |
| 1:D:87:THR:OG1 | 1:D:88:PRO:HD3 | 2.07 | 0.55 |
| 1:F:107:LEU:HD23 | 1:F:126:LYS:HE2 | 1.88 | 0.55 |
| 1:G:254:ASN:H | 1:G:257:LEU:HD12 | 1.69 | 0.55 |
| 1:G:358:LYS:HA | 1:G:361:LEU:HD22 | 1.86 | 0.55 |
| 1:K:195:HIS:O | 1:K:201:LYS:HE3 | 2.06 | 0.55 |
| 1:B:400:LYS:HB2 | 1:F:455:TYR:HB2 | 1.88 | 0.55 |
| 1:G:280:ILE:HD11 | 1:G:301:ILE:HD11 | 1.88 | 0.55 |
| 1:J:21:ALA:HB1 | 1:J:49:LEU:HD23 | 1.88 | 0.55 |
| 1:J:495:GLU:O | 1:K:177:SER:OG | 2.19 | 0.55 |
| 1:C:61:LEU:HD21 | 1:C:151:GLU:HB2 | 1.88 | 0.55 |
| 1:H:249:VAL:HG22 | 1:H:273:VAL:HG22 | 1.89 | 0.55 |
| 1:H:271:VAL:HG23 | 1:H:283:PRO:HA | 1.88 | 0.55 |
| 1:K:331:LEU:HB2 | 1:K:352:THR:HA | 1.89 | 0.55 |
| 1:C:211:ARG:HA | 1:C:214:ALA:HB2 | 1.87 | 0.55 |
| 1:K:217:ARG:NE | 1:K:450:HIS:ND1 | 2.55 | 0.55 |
| 1:J:227:ILE:HA | 1:J:233:MET:HE2 | 1.89 | 0.55 |
| 1:A:79:ARG:NH2 | 1:A:163:ASP:OD2 | 2.39 | 0.55 |
| 1:A:154:LYS:HE3 | 1:E:189:HIS:CD2 | 2.41 | 0.55 |
| 1:B:249:VAL:HA | 1:B:323:ILE:HG13 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:46:ARG:O | 1:C:50:ARG:HG3 | 2.07 | 0.55 |
| 1:B:280:ILE:HD11 | 1:B:301:ILE:HD11 | 1.90 | 0.54 |
| 1:D:383:PHE:HD1 | 1:D:449:VAL:HG13 | 1.72 | 0.54 |
| 1:I:65:ILE:HD13 | 1:I:144:ILE:HG12 | 1.90 | 0.54 |
| 1:J:46:ARG:O | 1:J:50:ARG:HG3 | 2.07 | 0.54 |
| 1:A:246:THR:HA | 1:A:269:LYS:O | 2.07 | 0.54 |
| 1:C:291:LEU:HD21 | 1:C:304:PHE:HB2 | 1.88 | 0.54 |
| 1:C:315:LEU:HD23 | 1:C:315:LEU:H | 1.72 | 0.54 |
| 1:H:107:LEU:HD23 | 1:H:126:LYS:HE2 | 1.87 | 0.54 |
| 1:K:94:ARG:NH1 | 1:K:103:GLU:OE2 | 2.40 | 0.54 |
| 1:B:118:VAL:HG23 | 1:B:120:VAL:HG23 | 1.90 | 0.54 |
| 1:B:193:ASN:HD22 | 1:B:389:LEU:CD2 | 2.20 | 0.54 |
| 1:C:242:PHE:HE2 | 1:C:266:PHE:HB3 | 1.71 | 0.54 |
| 1:F:303:GLY:O | 1:F:304:PHE:HD1 | 1.90 | 0.54 |
| 1:H:255:VAL:O | 1:H:259:SER:OG | 2.21 | 0.54 |
| 1:J:238:MET:HE3 | 1:J:342:LYS:HB2 | 1.88 | 0.54 |
| 1:D:303:GLY:O | 1:D:304:PHE:HD1 | 1.90 | 0.54 |
| 1:F:66:ARG:HD3 | 1:F:72:TRP:CE2 | 2.41 | 0.54 |
| 1:H:396:ARG:NH1 | 1:L:456:THR:OG1 | 2.40 | 0.54 |
| 1:A:6:ASP:OD1 | 1:A:6:ASP:N | 2.41 | 0.54 |
| 1:A:36:GLU:CG | 1:A:38:GLU:HG2 | 2.32 | 0.54 |
| 1:A:386:LEU:HD22 | 1:F:392:VAL:HG13 | 1.89 | 0.54 |
| 1:B:6:ASP:OD1 | 1:B:6:ASP:N | 2.41 | 0.54 |
| 1:B:421:PHE:CZ | 1:B:423:LYS:HB3 | 2.43 | 0.54 |
| 1:D:44:ARG:O | 1:D:48:ILE:HG12 | 2.08 | 0.54 |
| 1:D:195:HIS:O | 1:D:201:LYS:HE3 | 2.07 | 0.54 |
| 1:D:238:MET:HE3 | 1:D:342:LYS:HB2 | 1.90 | 0.54 |
| 1:F:65:ILE:HD13 | 1:F:144:ILE:HG12 | 1.89 | 0.54 |
| 1:F:89:CYS:HB3 | 1:F:125:ALA:HB2 | 1.88 | 0.54 |
| 1:I:332:THR:N | 1:I:335:ASN:OD1 | 2.31 | 0.54 |
| 1:L:168:ASP:N | 1:L:171:THR:OG1 | 2.33 | 0.54 |
| 1:A:91:GLY:HA3 | 1:A:125:ALA:O | 2.08 | 0.54 |
| 1:A:311:GLU:HG3 | 1:A:312:GLY:H | 1.73 | 0.54 |
| 1:C:89:CYS:HB3 | 1:C:125:ALA:HB2 | 1.90 | 0.54 |
| 1:C:242:PHE:CE2 | 1:C:266:PHE:HB3 | 2.43 | 0.54 |
| 1:C:294:PHE:CE2 | 1:C:301:ILE:HA | 2.43 | 0.54 |
| 1:D:181:ASP:O | 1:D:185:SER:OG | 2.21 | 0.54 |
| 1:G:195:HIS:CD2 | 1:H:87:THR:HG21 | 2.43 | 0.54 |
| 1:K:230:ALA:HA | 1:K:233:MET:HB2 | 1.89 | 0.54 |
| 1:A:186:THR:OG1 | 1:A:187:ILE:N | 2.41 | 0.54 |
| 1:B:198:VAL:O | 1:B:201:LYS:NZ | 2.35 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:414:GLN:HB2 | 1:C:429:PRO:HD2 | 1.89 | 0.54 |
| 1:K:242:PHE:HE2 | 1:K:266:PHE:HB3 | 1.73 | 0.54 |
| 1:A:319:CYS:SG | 1:A:320:ASP:N | 2.81 | 0.54 |
| 1:B:311:GLU:HG3 | 1:B:312:GLY:H | 1.73 | 0.54 |
| 1:I:259:SER:O | 1:I:263:LEU:HB2 | 2.08 | 0.54 |
| 1:I:324:PRO:HG2 | 1:I:351:PRO:HG2 | 1.90 | 0.54 |
| 1:K:298:HIS:CE1 | 1:K:304:PHE:CZ | 2.92 | 0.54 |
| 1:C:158:ILE:CD1 | 1:C:165:PRO:CD | 2.86 | 0.54 |
| 1:D:165:PRO:HD2 | 1:D:197:CYS:O | 2.08 | 0.54 |
| 1:G:195:HIS:O | 1:G:201:LYS:HE3 | 2.07 | 0.54 |
| 1:G:394:TYR:HB2 | 1:G:445:GLU:HG3 | 1.88 | 0.54 |
| 1:C:394:TYR:HB3 | 1:C:448:ILE:HD12 | 1.89 | 0.53 |
| 1:E:294:PHE:CE2 | 1:E:301:ILE:HG13 | 2.43 | 0.53 |
| 1:H:260:MET:HE2 | 1:H:288:PRO:HD3 | 1.89 | 0.53 |
| 1:I:165:PRO:HG2 | 1:I:198:VAL:HG23 | 1.90 | 0.53 |
| 1:J:90:LYS:HZ1 | 1:J:166:ALA:HB2 | 1.72 | 0.53 |
| 1:B:338:ARG:O | 1:B:363:ARG:NH1 | 2.41 | 0.53 |
| 1:D:277:ASP:OD2 | 1:D:300:THR:OG1 | 2.26 | 0.53 |
| 1:J:225:ASN:HD21 | 1:J:458:GLU:HA | 1.73 | 0.53 |
| 1:J:260:MET:HE2 | 1:J:288:PRO:HD3 | 1.89 | 0.53 |
| 1:B:427:THR:HG22 | 1:B:429:PRO:HD3 | 1.90 | 0.53 |
| 1:C:158:ILE:HD12 | 1:C:165:PRO:CD | 2.32 | 0.53 |
| 1:D:17:PHE:O | 1:D:21:ALA:N | 2.38 | 0.53 |
| 1:F:232:TYR:HB3 | 1:F:366:MET:HE1 | 1.91 | 0.53 |
| 1:H:79:ARG:HH11 | 1:H:127:ALA:HB2 | 1.73 | 0.53 |
| 1:C:44:ARG:O | 1:C:48:ILE:HG12 | 2.07 | 0.53 |
| 1:C:288:PRO:O | 1:C:292:GLU:HB3 | 2.08 | 0.53 |
| 1:F:107:LEU:HB3 | 1:F:126:LYS:HG2 | 1.88 | 0.53 |
| 1:D:414:GLN:HB2 | 1:D:429:PRO:HD2 | 1.90 | 0.53 |
| 1:D:498:VAL:O | 1:D:498:VAL:HG13 | 2.09 | 0.53 |
| 1:F:333:LYS:HE2 | 1:F:355:GLU:HG2 | 1.89 | 0.53 |
| 1:G:246:THR:HA | 1:G:269:LYS:O | 2.09 | 0.53 |
| 1:H:243:GLY:O | 1:H:245:LYS:N | 2.41 | 0.53 |
| 1:I:412:SER:HB3 | 1:K:432:PRO:HA | 1.90 | 0.53 |
| 1:K:25:GLU:OE2 | 1:K:46:ARG:NH2 | 2.42 | 0.53 |
| 1:K:61:LEU:HD21 | 1:K:151:GLU:HB3 | 1.88 | 0.53 |
| 1:L:399:PHE:CE1 | 1:L:443:ALA:HB1 | 2.43 | 0.53 |
| 1:B:396:ARG:NH1 | 1:F:456:THR:OG1 | 2.37 | 0.53 |
| 1:C:38:GLU:HB2 | 1:C:40:GLN:N | 2.22 | 0.53 |
| 1:D:38:GLU:HB3 | 1:D:40:GLN:H | 1.74 | 0.53 |
| 1:J:90:LYS:NZ | 1:J:166:ALA:HB2 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:498:VAL:HB | 1:F:72:TRP:HH2 | 1.72 | 0.53 |
| 1:F:93:ILE:HG22 | 1:F:127:ALA:HB3 | 1.89 | 0.53 |
| 1:H:352:THR:HG21 | 1:H:357:ASP:OD1 | 2.08 | 0.53 |
| 1:I:91:GLY:HA3 | 1:I:125:ALA:O | 2.09 | 0.53 |
| 1:K:414:GLN:OE1 | 1:K:429:PRO:HD2 | 2.09 | 0.53 |
| 1:E:52:ILE:HG12 | 1:E:493:TYR:HE2 | 1.73 | 0.53 |
| 1:E:348:ALA:HB3 | 1:E:351:PRO:HG3 | 1.89 | 0.53 |
| 1:G:298:HIS:CE1 | 1:G:304:PHE:HZ | 2.26 | 0.53 |
| 1:L:91:GLY:HA3 | 1:L:125:ALA:O | 2.09 | 0.53 |
| 1:A:385:TRP:O | 1:A:389:LEU:HG | 2.09 | 0.53 |
| 1:G:8:ASN:O | 1:G:329:LYS:NZ | 2.38 | 0.53 |
| 1:J:93:ILE:HD11 | 1:J:176:MET:HE1 | 1.91 | 0.53 |
| 1:K:433:THR:HG23 | 1:K:436:PHE:H | 1.71 | 0.53 |
| 1:J:455:TYR:HB2 | 1:K:400:LYS:HB2 | 1.91 | 0.53 |
| 1:A:345:ALA:HB1 | 1:A:373:LEU:HD22 | 1.91 | 0.52 |
| 1:K:141:LEU:O | 1:K:145:THR:HG23 | 2.09 | 0.52 |
| 1:K:305:PRO:C | 1:K:307:ALA:H | 2.17 | 0.52 |
| 1:L:141:LEU:O | 1:L:145:THR:HG23 | 2.08 | 0.52 |
| 1:A:13:VAL:HA | 1:A:16:PHE:CD2 | 2.44 | 0.52 |
| 1:G:141:LEU:O | 1:G:145:THR:HG23 | 2.09 | 0.52 |
| 1:I:94:ARG:NE | 1:I:169:MET:HG3 | 2.24 | 0.52 |
| 1:I:321:ILE:HG12 | 1:I:343:ILE:HG23 | 1.91 | 0.52 |
| 1:K:246:THR:HA | 1:K:269:LYS:O | 2.08 | 0.52 |
| 1:L:321:ILE:HG12 | 1:L:343:ILE:HG23 | 1.91 | 0.52 |
| 1:G:382:TYR:O | 1:G:386:LEU:HG | 2.09 | 0.52 |
| 1:K:131:ILE:HB | 1:K:136:TYR:HE2 | 1.73 | 0.52 |
| 1:C:87:THR:OG1 | 1:C:88:PRO:HD3 | 2.10 | 0.52 |
| 1:E:219:VAL:HA | 1:E:373:LEU:HG | 1.91 | 0.52 |
| 1:E:316:GLU:HA | 1:E:339:VAL:HA | 1.92 | 0.52 |
| 1:I:282:ASN:HD21 | 1:I:306:LYS:HB2 | 1.74 | 0.52 |
| 1:K:16:PHE:CZ | 1:K:354:PRO:HD3 | 2.45 | 0.52 |
| 1:L:260:MET:HE3 | 1:L:288:PRO:HB3 | 1.90 | 0.52 |
| 1:E:224:GLU:O | 1:E:228:ASN:HB2 | 2.10 | 0.52 |
| 1:K:87:THR:OG1 | 1:K:88:PRO:HD3 | 2.09 | 0.52 |
| 1:B:294:PHE:CD1 | 1:B:298:HIS:CE1 | 2.90 | 0.52 |
| 1:C:366:MET:CE | 1:C:475:LEU:HD23 | 2.30 | 0.52 |
| 1:E:52:ILE:HG12 | 1:E:493:TYR:CE2 | 2.45 | 0.52 |
| 1:E:335:ASN:OD1 | 1:E:335:ASN:N | 2.43 | 0.52 |
| 1:I:343:ILE:HD11 | 1:I:368:ILE:HD11 | 1.92 | 0.52 |
| 1:D:270:CYS:SG | 1:D:271:VAL:N | 2.83 | 0.52 |
| 1:E:186:THR:OG1 | 1:E:187:ILE:N | 2.37 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:95:TYR:OH | 1:G:145:THR:HG22 | 2.09 | 0.52 |
| 1:B:229:GLU:HG3 | 1:B:465:MET:HE1 | 1.92 | 0.52 |
| 1:F:459:ARG:NH2 | 2:F:601:XEG:OAH | 2.37 | 0.52 |
| 1:I:230:ALA:HA | 1:I:233:MET:HB2 | 1.92 | 0.52 |
| 1:J:141:LEU:O | 1:J:145:THR:HG23 | 2.10 | 0.52 |
| 1:J:420:LYS:HG3 | 1:J:421:PHE:N | 2.25 | 0.52 |
| 1:C:52:ILE:O | 1:C:82:HIS:NE2 | 2.42 | 0.52 |
| 1:C:259:SER:O | 1:C:263:LEU:HB2 | 2.10 | 0.52 |
| 1:D:67:ARG:NH2 | 1:D:135:ASN:O | 2.43 | 0.52 |
| 1:F:131:ILE:HB | 1:F:136:TYR:HE2 | 1.74 | 0.52 |
| 1:H:324:PRO:HG2 | 1:H:351:PRO:HG2 | 1.92 | 0.52 |
| 1:I:58:VAL:CG1 | 1:L:60:SER:HB2 | 2.40 | 0.52 |
| 1:K:83:SER:OG | 1:K:85:HIS:ND1 | 2.33 | 0.52 |
| 1:E:126:LYS:NZ | 1:E:168:ASP:OD2 | 2.24 | 0.51 |
| 1:H:142:GLU:HG3 | 1:H:178:TRP:CE2 | 2.45 | 0.51 |
| 1:K:246:THR:OG1 | 1:K:271:VAL:HB | 2.10 | 0.51 |
| 1:A:34:THR:HG23 | 1:A:36:GLU:HB3 | 1.93 | 0.51 |
| 1:B:112:THR:OG1 | 1:B:124:GLY:HA3 | 2.11 | 0.51 |
| 1:E:152:LEU:HB3 | 1:E:157:PHE:HB2 | 1.92 | 0.51 |
| 1:I:255:VAL:O | 1:I:259:SER:OG | 2.14 | 0.51 |
| 1:A:281:TRP:CD1 | 1:A:310:TYR:CD1 | 2.98 | 0.51 |
| 1:A:412:SER:HB3 | 1:B:432:PRO:HA | 1.91 | 0.51 |
| 1:B:93:ILE:HD11 | 1:B:176:MET:HE1 | 1.92 | 0.51 |
| 1:E:260:MET:HE1 | 1:E:286:ILE:HD11 | 1.90 | 0.51 |
| 1:F:51:ILE:O | 1:F:54:PRO:HD2 | 2.10 | 0.51 |
| 1:F:158:ILE:CD1 | 1:F:165:PRO:CD | 2.88 | 0.51 |
| 1:G:357:ASP:O | 1:G:361:LEU:HD22 | 2.10 | 0.51 |
| 1:I:242:PHE:HE2 | 1:I:266:PHE:HB3 | 1.76 | 0.51 |
| 1:I:294:PHE:HE2 | 1:I:302:LEU:H | 1.57 | 0.51 |
| 1:J:421:PHE:HZ | 1:J:423:LYS:HE3 | 1.75 | 0.51 |
| 1:B:165:PRO:HD2 | 1:B:197:CYS:O | 2.10 | 0.51 |
| 1:B:414:GLN:OE1 | 1:B:430:ILE:HG12 | 2.10 | 0.51 |
| 1:C:275:GLU:HG2 | 1:C:276:SER:H | 1.75 | 0.51 |
| 1:G:433:THR:HG23 | 1:G:436:PHE:H | 1.75 | 0.51 |
| 1:I:119:ASP:O | 1:J:396:ARG:NH2 | 2.40 | 0.51 |
| 1:K:8:ASN:HA | 1:K:329:LYS:HE3 | 1.92 | 0.51 |
| 1:D:280:ILE:HD13 | 1:D:307:ALA:HB1 | 1.92 | 0.51 |
| 1:E:462:ARG:O | 1:E:466:ARG:HG2 | 2.10 | 0.51 |
| 1:G:19:ARG:HH11 | 1:G:479:THR:HG21 | 1.74 | 0.51 |
| 1:G:275:GLU:HG2 | 1:G:276:SER:N | 2.21 | 0.51 |
| 1:I:142:GLU:HG3 | 1:I:178:TRP:CE2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:16:PHE:CE1 | 1:A:354:PRO:HD3 | 2.46 | 0.51 |
| 1:A:279:SER:HB3 | 1:A:310:TYR:HB3 | 1.93 | 0.51 |
| 1:C:303:GLY:O | 1:C:304:PHE:CD1 | 2.62 | 0.51 |
| 1:D:281:TRP:CZ3 | 1:D:317:VAL:HG13 | 2.46 | 0.51 |
| 1:H:394:TYR:HB2 | 1:H:445:GLU:HG3 | 1.92 | 0.51 |
| 1:A:141:LEU:O | 1:A:145:THR:HG23 | 2.11 | 0.51 |
| 1:A:165:PRO:HG2 | 1:A:198:VAL:HG23 | 1.91 | 0.51 |
| 1:B:382:TYR:CE1 | 1:B:386:LEU:HD11 | 2.46 | 0.51 |
| 1:J:298:HIS:CE1 | 1:J:304:PHE:HZ | 2.29 | 0.51 |
| 1:L:304:PHE:H | 1:L:307:ALA:HB3 | 1.75 | 0.51 |
| 1:E:288:PRO:O | 1:E:292:GLU:HB3 | 2.10 | 0.51 |
| 1:J:254:ASN:H | 1:J:257:LEU:HD12 | 1.76 | 0.51 |
| 1:E:238:MET:HE1 | 1:E:343:ILE:HG22 | 1.92 | 0.51 |
| 1:G:118:VAL:HG23 | 1:G:120:VAL:HG23 | 1.92 | 0.51 |
| 1:I:175:GLU:O | 1:I:179:ILE:HG13 | 2.11 | 0.51 |
| 1:K:116:ALA:HA | 2:K:601:XEG:OAC | 2.11 | 0.51 |
| 1:C:291:LEU:HD11 | 1:C:307:ALA:HB2 | 1.93 | 0.51 |
| 1:D:118:VAL:HG23 | 1:D:120:VAL:HG23 | 1.93 | 0.51 |
| 1:F:238:MET:HE3 | 1:F:342:LYS:HB2 | 1.93 | 0.51 |
| 1:F:259:SER:O | 1:F:263:LEU:HB2 | 2.10 | 0.51 |
| 1:F:281:TRP:CZ3 | 1:F:317:VAL:HG13 | 2.46 | 0.51 |
| 1:I:221:HIS:O | 1:I:225:ASN:ND2 | 2.44 | 0.51 |
| 1:I:337:PRO:O | 1:I:363:ARG:NH2 | 2.43 | 0.51 |
| 1:I:477:LEU:HA | 1:I:480:ALA:HB3 | 1.91 | 0.51 |
| 1:B:44:ARG:O | 1:B:48:ILE:HG12 | 2.11 | 0.50 |
| 1:B:319:CYS:SG | 1:B:320:ASP:N | 2.84 | 0.50 |
| 1:G:277:ASP:OD2 | 1:G:300:THR:HG21 | 2.11 | 0.50 |
| 1:B:498:VAL:HG13 | 1:B:498:VAL:O | 2.11 | 0.50 |
| 1:D:433:THR:HG23 | 1:D:436:PHE:H | 1.76 | 0.50 |
| 1:G:242:PHE:HE2 | 1:G:266:PHE:HB3 | 1.76 | 0.50 |
| 1:C:131:ILE:HB | 1:C:136:TYR:HE2 | 1.75 | 0.50 |
| 1:C:164:VAL:HG13 | 1:C:198:VAL:HA | 1.93 | 0.50 |
| 1:D:303:GLY:O | 1:D:304:PHE:CD1 | 2.64 | 0.50 |
| 1:E:165:PRO:HD2 | 1:E:197:CYS:O | 2.12 | 0.50 |
| 1:E:168:ASP:OD1 | 1:E:169:MET:N | 2.44 | 0.50 |
| 1:G:213:SER:HB3 | 1:G:262:TYR:HE2 | 1.77 | 0.50 |
| 1:J:480:ALA:CA | 1:J:483:VAL:HG12 | 2.42 | 0.50 |
| 1:K:119:ASP:HA | 2:K:601:XEG:HAI | 1.91 | 0.50 |
| 1:A:313:SER:OG | 1:A:316:GLU:HG2 | 2.11 | 0.50 |
| 1:C:274:GLY:HA2 | 1:C:279:SER:HA | 1.93 | 0.50 |
| 1:F:141:LEU:O | 1:F:145:THR:HG23 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:186:THR:OG1 | 1:B:187:ILE:N | 2.45 | 0.50 |
| 1:C:270:CYS:SG | 1:C:271:VAL:N | 2.84 | 0.50 |
| 1:C:315:LEU:HD12 | 1:C:339:VAL:HG22 | 1.93 | 0.50 |
| 1:D:21:ALA:HB1 | 1:D:49:LEU:HD23 | 1.94 | 0.50 |
| 1:E:250:GLN:NE2 | 1:E:330:GLN:HE21 | 2.09 | 0.50 |
| 1:F:335:ASN:N | 1:F:335:ASN:OD1 | 2.44 | 0.50 |
| 1:F:484:ASN:O | 1:F:487:GLU:HG2 | 2.11 | 0.50 |
| 1:I:219:VAL:HA | 1:I:373:LEU:HG | 1.93 | 0.50 |
| 1:I:294:PHE:HD2 | 1:I:301:ILE:HD12 | 1.76 | 0.50 |
| 1:I:463:GLN:OE1 | 1:I:488:LYS:NZ | 2.38 | 0.50 |
| 1:A:281:TRP:HD1 | 1:A:310:TYR:CD1 | 2.30 | 0.50 |
| 1:D:36:GLU:O | 1:D:37:THR:OG1 | 2.25 | 0.50 |
| 1:F:281:TRP:HZ3 | 1:F:317:VAL:HG13 | 1.77 | 0.50 |
| 1:F:337:PRO:O | 1:F:363:ARG:NH2 | 2.45 | 0.50 |
| 1:G:383:PHE:HA | 1:G:386:LEU:HD12 | 1.93 | 0.50 |
| 1:H:6:ASP:N | 1:H:7:PRO:HD3 | 2.27 | 0.50 |
| 1:H:473:LEU:O | 1:H:475:LEU:N | 2.44 | 0.50 |
| 1:L:346:GLU:CD | 1:L:478:ARG:HH12 | 2.20 | 0.50 |
| 1:A:151:GLU:OE1 | 1:D:57:HIS:NE2 | 2.39 | 0.50 |
| 1:B:213:SER:HA | 1:B:258:HIS:ND1 | 2.27 | 0.50 |
| 1:C:396:ARG:NH1 | 1:E:456:THR:OG1 | 2.38 | 0.50 |
| 1:G:13:VAL:O | 1:G:16:PHE:N | 2.43 | 0.50 |
| 1:G:378:VAL:HA | 1:G:381:SER:HB2 | 1.94 | 0.50 |
| 1:I:291:LEU:CD1 | 1:I:304:PHE:CD2 | 2.95 | 0.50 |
| 1:J:271:VAL:HG23 | 1:J:283:PRO:HA | 1.94 | 0.50 |
| 1:K:421:PHE:HZ | 1:K:423:LYS:HE3 | 1.76 | 0.50 |
| 1:C:335:ASN:N | 1:C:335:ASN:OD1 | 2.44 | 0.50 |
| 1:F:332:THR:OG1 | 1:F:355:GLU:OE1 | 2.21 | 0.50 |
| 1:I:186:THR:OG1 | 1:I:187:ILE:N | 2.45 | 0.50 |
| 1:A:9:PHE:CD2 | 1:A:329:LYS:NZ | 2.76 | 0.50 |
| 1:A:11:LYS:HG3 | 1:A:14:GLU:CB | 2.41 | 0.50 |
| 1:A:60:SER:HB2 | 1:D:58:VAL:HG13 | 1.94 | 0.50 |
| 1:A:99:VAL:O | 1:A:130:LYS:HE2 | 2.12 | 0.50 |
| 1:B:327:SER:HB3 | 1:B:330:GLN:NE2 | 2.25 | 0.50 |
| 1:K:323:ILE:HA | 1:K:345:ALA:O | 2.12 | 0.50 |
| 1:B:303:GLY:O | 1:B:304:PHE:CD1 | 2.64 | 0.49 |
| 1:B:315:LEU:HD13 | 1:B:335:ASN:HD22 | 1.77 | 0.49 |
| 1:D:294:PHE:CD2 | 1:D:301:ILE:HD12 | 2.47 | 0.49 |
| 1:E:343:ILE:HA | 1:E:366:MET:HB3 | 1.93 | 0.49 |
| 1:G:499:THR:HG22 | 1:G:501:THR:HG23 | 1.94 | 0.49 |
| 1:J:213:SER:HB3 | 1:J:262:TYR:CE2 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:61:LEU:HD21 | 1:L:151:GLU:CB | 2.42 | 0.49 |
| 1:C:238:MET:HG3 | 1:C:245:LYS:HZ3 | 1.76 | 0.49 |
| 1:D:91:GLY:HA3 | 1:D:125:ALA:O | 2.12 | 0.49 |
| 1:D:333:LYS:HG3 | 1:D:355:GLU:HG2 | 1.94 | 0.49 |
| 1:E:91:GLY:HA3 | 1:E:125:ALA:O | 2.12 | 0.49 |
| 1:E:94:ARG:HD3 | 1:E:169:MET:HB3 | 1.93 | 0.49 |
| 1:E:141:LEU:O | 1:E:145:THR:HG23 | 2.12 | 0.49 |
| 1:E:251:GLY:O | 1:E:253:GLY:N | 2.45 | 0.49 |
| 1:E:274:GLY:HA3 | 1:E:314:ILE:HD13 | 1.94 | 0.49 |
| 1:L:6:ASP:HB2 | 1:L:332:THR:HG21 | 1.95 | 0.49 |
| 1:L:85:HIS:CD2 | 1:L:86:ARG:HG2 | 2.46 | 0.49 |
| 1:B:47:GLY:O | 1:B:51:ILE:HG13 | 2.12 | 0.49 |
| 1:C:66:ARG:HH11 | 1:F:498:VAL:HG11 | 1.76 | 0.49 |
| 1:C:412:SER:HB3 | 1:E:432:PRO:HA | 1.94 | 0.49 |
| 1:F:66:ARG:HD3 | 1:F:72:TRP:CZ2 | 2.47 | 0.49 |
| 1:H:208:ILE:H | 1:H:211:ARG:HE | 1.59 | 0.49 |
| 1:J:227:ILE:HD12 | 1:J:242:PHE:HD1 | 1.76 | 0.49 |
| 1:J:335:ASN:OD1 | 1:J:335:ASN:N | 2.45 | 0.49 |
| 1:A:66:ARG:HD3 | 1:A:72:TRP:CE2 | 2.47 | 0.49 |
| 1:C:382:TYR:O | 1:C:386:LEU:HG | 2.13 | 0.49 |
| 1:D:304:PHE:H | 1:D:307:ALA:HB3 | 1.77 | 0.49 |
| 1:F:82:HIS:CG | 1:F:109:SER:HA | 2.47 | 0.49 |
| 1:J:79:ARG:HH21 | 1:J:163:ASP:CG | 2.20 | 0.49 |
| 1:J:338:ARG:O | 1:J:363:ARG:NH1 | 2.45 | 0.49 |
| 1:J:372:TYR:OH | 1:J:461:ALA:HB2 | 2.12 | 0.49 |
| 1:K:329:LYS:H | 1:K:351:PRO:HA | 1.76 | 0.49 |
| 1:B:412:SER:HB3 | 1:F:432:PRO:HA | 1.94 | 0.49 |
| 1:E:378:VAL:HA | 1:E:381:SER:HB2 | 1.95 | 0.49 |
| 1:F:38:GLU:HB2 | 1:F:40:GLN:H | 1.75 | 0.49 |
| 1:H:224:GLU:O | 1:H:228:ASN:HB2 | 2.11 | 0.49 |
| 1:H:311:GLU:HG3 | 1:H:312:GLY:H | 1.78 | 0.49 |
| 1:L:16:PHE:CZ | 1:L:354:PRO:HD3 | 2.48 | 0.49 |
| 1:A:209:HIS:HB3 | 1:A:446:LYS:HB3 | 1.95 | 0.49 |
| 1:A:251:GLY:O | 1:A:253:GLY:N | 2.46 | 0.49 |
| 1:A:327:SER:OG | 1:A:328:GLU:N | 2.45 | 0.49 |
| 1:C:421:PHE:CE1 | 1:C:423:LYS:HB2 | 2.47 | 0.49 |
| 1:E:275:GLU:HG2 | 1:E:276:SER:H | 1.77 | 0.49 |
| 1:F:208:ILE:H | 1:F:211:ARG:HH11 | 1.60 | 0.49 |
| 1:G:186:THR:OG1 | 1:G:187:ILE:N | 2.43 | 0.49 |
| 1:G:208:ILE:O | 1:G:211:ARG:NH1 | 2.45 | 0.49 |
| 1:J:473:LEU:O | 1:J:475:LEU:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:57:HIS:NE2 | 1:J:151:GLU:HG3 | 2.27 | 0.49 |
| 1:H:303:GLY:O | 1:H:304:PHE:HD1 | 1.94 | 0.49 |
| 1:K:499:THR:HG22 | 1:K:501:THR:HG23 | 1.94 | 0.49 |
| 1:B:6:ASP:N | 1:B:355:GLU:OE1 | 2.45 | 0.49 |
| 1:B:62:SER:HB3 | 1:E:56:ASN:HA | 1.93 | 0.49 |
| 1:B:249:VAL:CG1 | 1:B:323:ILE:HD11 | 2.34 | 0.49 |
| 1:E:382:TYR:CZ | 1:E:386:LEU:HD11 | 2.48 | 0.49 |
| 1:G:213:SER:HB3 | 1:G:262:TYR:CE2 | 2.48 | 0.49 |
| 1:A:224:GLU:O | 1:A:228:ASN:HB2 | 2.12 | 0.49 |
| 1:B:87:THR:OG1 | 1:B:88:PRO:HD3 | 2.11 | 0.49 |
| 1:C:94:ARG:NH1 | 1:C:103:GLU:OE2 | 2.46 | 0.49 |
| 1:J:113:TYR:HB2 | 1:J:371:LEU:HD11 | 1.94 | 0.49 |
| 1:K:382:TYR:O | 1:K:386:LEU:HG | 2.12 | 0.49 |
| 1:E:38:GLU:HG3 | 1:E:40:GLN:H | 1.77 | 0.49 |
| 1:E:370:ASP:OD1 | 1:E:478:ARG:NH1 | 2.45 | 0.49 |
| 1:G:36:GLU:OE1 | 1:G:41:LYS:HG2 | 2.13 | 0.49 |
| 1:G:253:GLY:O | 1:G:255:VAL:N | 2.45 | 0.49 |
| 1:G:329:LYS:H | 1:G:351:PRO:HA | 1.78 | 0.49 |
| 1:H:378:VAL:HA | 1:H:381:SER:HB2 | 1.93 | 0.49 |
| 1:I:201:LYS:NZ | 1:I:384:GLU:OE1 | 2.40 | 0.49 |
| 1:L:332:THR:OG1 | 1:L:333:LYS:N | 2.39 | 0.49 |
| 1:A:382:TYR:CE1 | 1:A:386:LEU:HD11 | 2.47 | 0.48 |
| 1:B:140:GLU:O | 1:B:144:ILE:HG13 | 2.13 | 0.48 |
| 1:D:315:LEU:HB3 | 1:D:322:LEU:HD21 | 1.95 | 0.48 |
| 1:F:220:PHE:CZ | 1:F:266:PHE:HE2 | 2.31 | 0.48 |
| 1:G:88:PRO:HG2 | 1:G:122:PHE:CE2 | 2.48 | 0.48 |
| 1:I:193:ASN:HD22 | 1:I:389:LEU:HA | 1.78 | 0.48 |
| 1:J:232:TYR:HD1 | 1:J:235:ILE:HD12 | 1.77 | 0.48 |
| 1:D:249:VAL:HA | 1:D:323:ILE:HG13 | 1.95 | 0.48 |
| 1:D:281:TRP:HZ3 | 1:D:317:VAL:HG13 | 1.77 | 0.48 |
| 1:H:72:TRP:CH2 | 1:K:498:VAL:HB | 2.47 | 0.48 |
| 1:I:60:SER:HB2 | 1:L:58:VAL:CG1 | 2.43 | 0.48 |
| 1:K:53:LYS:HG3 | 1:K:54:PRO:HD3 | 1.95 | 0.48 |
| 1:H:205:GLN:NE2 | 1:L:492:VAL:O | 2.47 | 0.48 |
| 1:H:382:TYR:CZ | 1:H:386:LEU:HD11 | 2.48 | 0.48 |
| 1:A:282:ASN:ND2 | 1:A:306:LYS:HB3 | 2.28 | 0.48 |
| 1:D:490:PHE:HE2 | 1:D:494:ASN:HD22 | 1.61 | 0.48 |
| 1:E:226:PHE:C | 1:E:228:ASN:H | 2.22 | 0.48 |
| 1:E:270:CYS:SG | 1:E:271:VAL:N | 2.86 | 0.48 |
| 1:H:195:HIS:O | 1:H:201:LYS:HE3 | 2.12 | 0.48 |
| 1:J:52:ILE:HD13 | 1:J:489:VAL:HG12 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:300:THR:HG22 | 1:K:301:ILE:H | 1.79 | 0.48 |
| 1:L:280:ILE:HD13 | 1:L:307:ALA:HB1 | 1.95 | 0.48 |
| 1:B:27:LYS:HA | 1:B:30:GLU:HB2 | 1.96 | 0.48 |
| 1:C:282:ASN:ND2 | 1:C:306:LYS:O | 2.43 | 0.48 |
| 1:K:321:ILE:HA | 1:K:343:ILE:O | 2.13 | 0.48 |
| 1:A:335:ASN:N | 1:A:335:ASN:OD1 | 2.46 | 0.48 |
| 1:G:87:THR:CG2 | 1:G:88:PRO:HD3 | 2.39 | 0.48 |
| 1:H:202:PRO:HA | 1:H:211:ARG:HH22 | 1.78 | 0.48 |
| 1:H:335:ASN:N | 1:H:335:ASN:OD1 | 2.47 | 0.48 |
| 1:I:85:HIS:CB | 1:I:493:TYR:HE1 | 2.19 | 0.48 |
| 1:K:379:THR:O | 1:K:382:TYR:HB3 | 2.14 | 0.48 |
| 1:L:445:GLU:O | 1:L:449:VAL:HG23 | 2.13 | 0.48 |
| 1:A:427:THR:HG22 | 1:A:429:PRO:HD3 | 1.95 | 0.48 |
| 1:G:91:GLY:HA3 | 1:G:125:ALA:O | 2.14 | 0.48 |
| 1:J:294:PHE:CE2 | 1:J:301:ILE:HA | 2.48 | 0.48 |
| 1:K:8:ASN:OD1 | 1:K:9:PHE:N | 2.47 | 0.48 |
| 1:L:220:PHE:O | 1:L:224:GLU:N | 2.45 | 0.48 |
| 1:B:335:ASN:OD1 | 1:B:335:ASN:N | 2.47 | 0.48 |
| 1:C:202:PRO:HG2 | 1:C:205:GLN:HG3 | 1.96 | 0.48 |
| 1:H:202:PRO:HG2 | 1:H:205:GLN:HG3 | 1.96 | 0.48 |
| 1:I:291:LEU:HD11 | 1:I:304:PHE:CD2 | 2.49 | 0.48 |
| 1:I:496:ALA:HB2 | 1:J:205:GLN:HE22 | 1.78 | 0.48 |
| 1:L:459:ARG:NH2 | 2:L:601:XEG:OAH | 2.42 | 0.48 |
| 1:I:303:GLY:O | 1:I:304:PHE:CD1 | 2.67 | 0.48 |
| 1:A:244:ASP:OD1 | 1:A:244:ASP:N | 2.45 | 0.48 |
| 1:B:10:PHE:O | 1:B:12:MET:N | 2.45 | 0.48 |
| 1:B:315:LEU:CD1 | 1:B:335:ASN:HD22 | 2.26 | 0.48 |
| 1:B:315:LEU:HD12 | 1:B:339:VAL:HG22 | 1.95 | 0.48 |
| 1:C:263:LEU:HD12 | 1:C:263:LEU:HA | 1.69 | 0.48 |
| 1:E:45:VAL:HG22 | 1:E:490:PHE:CZ | 2.49 | 0.48 |
| 1:E:319:CYS:SG | 1:E:320:ASP:N | 2.84 | 0.48 |
| 1:H:279:SER:HB3 | 1:H:314:ILE:HG12 | 1.95 | 0.48 |
| 1:J:421:PHE:CZ | 1:J:423:LYS:HE3 | 2.49 | 0.48 |
| 1:L:350:GLY:N | 1:L:370:ASP:OD2 | 2.45 | 0.48 |
| 1:B:280:ILE:HD13 | 1:B:307:ALA:HB1 | 1.95 | 0.47 |
| 1:C:421:PHE:CZ | 1:C:423:LYS:HB2 | 2.49 | 0.47 |
| 1:D:95:TYR:OH | 1:D:145:THR:HG22 | 2.13 | 0.47 |
| 1:H:94:ARG:NH1 | 1:H:103:GLU:OE2 | 2.46 | 0.47 |
| 2:C:601:XEG:OAF | 1:D:396:ARG:NE | 2.35 | 0.47 |
| 1:E:444:SER:N | 1:E:447:ASP:OD2 | 2.43 | 0.47 |
| 1:J:305:PRO:C | 1:J:307:ALA:H | 2.22 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:303:GLY:O | 1:K:304:PHE:CD1 | 2.65 | 0.47 |
| 1:L:368:ILE:HG21 | 1:L:373:LEU:HD13 | 1.96 | 0.47 |
| 1:A:227:ILE:HA | 1:A:233:MET:HE3 | 1.95 | 0.47 |
| 1:B:13:VAL:O | 1:B:16:PHE:N | 2.47 | 0.47 |
| 1:B:249:VAL:HG12 | 1:B:323:ILE:CD1 | 2.32 | 0.47 |
| 1:C:319:CYS:SG | 1:C:320:ASP:N | 2.87 | 0.47 |
| 1:C:433:THR:HG23 | 1:C:436:PHE:H | 1.78 | 0.47 |
| 1:D:246:THR:HA | 1:D:269:LYS:O | 2.14 | 0.47 |
| 1:D:329:LYS:H | 1:D:351:PRO:HA | 1.79 | 0.47 |
| 1:E:248:ALA:HB1 | 1:E:272:ALA:HB3 | 1.95 | 0.47 |
| 1:E:459:ARG:NH1 | 2:E:601:XEG:OAH | 2.38 | 0.47 |
| 1:H:372:TYR:OH | 1:H:461:ALA:HB2 | 2.12 | 0.47 |
| 1:I:213:SER:HB3 | 1:I:262:TYR:HE2 | 1.79 | 0.47 |
| 1:I:242:PHE:CE2 | 1:I:266:PHE:HB3 | 2.50 | 0.47 |
| 1:J:87:THR:HG23 | 1:J:88:PRO:CD | 2.32 | 0.47 |
| 1:B:250:GLN:HG3 | 1:B:314:ILE:HD12 | 1.95 | 0.47 |
| 1:C:260:MET:HE2 | 1:C:288:PRO:HB3 | 1.96 | 0.47 |
| 1:D:85:HIS:CD2 | 1:D:86:ARG:HG2 | 2.49 | 0.47 |
| 1:D:140:GLU:O | 1:D:144:ILE:HG13 | 2.15 | 0.47 |
| 1:F:44:ARG:O | 1:F:48:ILE:HG12 | 2.14 | 0.47 |
| 1:F:303:GLY:O | 1:F:304:PHE:CD1 | 2.67 | 0.47 |
| 1:G:217:ARG:NE | 1:G:450:HIS:CD2 | 2.82 | 0.47 |
| 2:I:601:XEG:OAF | 1:J:396:ARG:NE | 2.40 | 0.47 |
| 1:L:291:LEU:HD11 | 1:L:304:PHE:HB2 | 1.96 | 0.47 |
| 1:A:304:PHE:CG | 1:A:305:PRO:HD3 | 2.48 | 0.47 |
| 1:E:473:LEU:O | 1:E:475:LEU:N | 2.48 | 0.47 |
| 1:G:9:PHE:HD1 | 1:G:10:PHE:N | 2.12 | 0.47 |
| 1:G:52:ILE:HG12 | 1:G:493:TYR:CE2 | 2.48 | 0.47 |
| 1:G:303:GLY:O | 1:G:304:PHE:CD1 | 2.67 | 0.47 |
| 1:H:361:LEU:O | 1:H:361:LEU:HD12 | 2.15 | 0.47 |
| 1:J:211:ARG:HA | 1:J:214:ALA:HB2 | 1.95 | 0.47 |
| 1:J:213:SER:HA | 1:J:258:HIS:ND1 | 2.29 | 0.47 |
| 1:A:193:ASN:HD22 | 1:A:389:LEU:HA | 1.79 | 0.47 |
| 1:F:369:PRO:HB3 | 1:F:478:ARG:HG3 | 1.97 | 0.47 |
| 1:B:151:GLU:HG3 | 1:E:57:HIS:NE2 | 2.30 | 0.47 |
| 1:B:195:HIS:O | 1:B:201:LYS:HE3 | 2.14 | 0.47 |
| 1:B:311:GLU:HG3 | 1:B:312:GLY:N | 2.30 | 0.47 |
| 1:C:91:GLY:HA3 | 1:C:125:ALA:O | 2.14 | 0.47 |
| 1:C:129:VAL:HG12 | 1:C:131:ILE:HG12 | 1.94 | 0.47 |
| 1:E:246:THR:HA | 1:E:269:LYS:O | 2.14 | 0.47 |
| 1:F:200:GLY:H | 1:F:384:GLU:CD | 2.23 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:601:XEG:HBE | 2:F:601:XEG:HAJ | 1.49 | 0.47 |
| 1:H:91:GLY:HA3 | 1:H:125:ALA:O | 2.14 | 0.47 |
| 1:I:227:ILE:HG23 | 1:I:233:MET:HE3 | 1.96 | 0.47 |
| 2:K:601:XEG:HBE | 2:K:601:XEG:HAJ | 1.44 | 0.47 |
| 1:L:219:VAL:HA | 1:L:373:LEU:HG | 1.95 | 0.47 |
| 1:L:251:GLY:HA3 | 1:L:326:ALA:HB2 | 1.97 | 0.47 |
| 1:L:251:GLY:O | 1:L:253:GLY:N | 2.48 | 0.47 |
| 1:A:372:TYR:OH | 1:A:461:ALA:HB2 | 2.14 | 0.47 |
| 1:G:131:ILE:HB | 1:G:136:TYR:CE2 | 2.49 | 0.47 |
| 1:H:138:ASP:OD2 | 1:L:35:ARG:NH1 | 2.48 | 0.47 |
| 1:I:236:LEU:HD21 | 1:I:342:LYS:HG3 | 1.97 | 0.47 |
| 1:L:259:SER:O | 1:L:263:LEU:HB2 | 2.15 | 0.47 |
| 1:A:219:VAL:HA | 1:A:373:LEU:HG | 1.97 | 0.47 |
| 1:A:382:TYR:CZ | 1:A:386:LEU:HD11 | 2.49 | 0.47 |
| 1:B:322:LEU:O | 1:B:344:ILE:HA | 2.15 | 0.47 |
| 1:E:37:THR:HA | 1:E:41:LYS:HE3 | 1.97 | 0.47 |
| 1:H:419:ARG:NH1 | 1:L:431:VAL:HG11 | 2.30 | 0.47 |
| 1:H:419:ARG:HH12 | 1:L:431:VAL:HG11 | 1.80 | 0.47 |
| 1:I:220:PHE:O | 1:I:224:GLU:N | 2.42 | 0.47 |
| 1:I:297:GLN:O | 1:I:298:HIS:ND1 | 2.44 | 0.47 |
| 1:K:150:MET:HE3 | 1:K:150:MET:HB3 | 1.71 | 0.47 |
| 1:K:346:GLU:OE1 | 1:K:478:ARG:NH1 | 2.48 | 0.47 |
| 1:A:8:ASN:HB3 | 1:A:9:PHE:CD2 | 2.50 | 0.47 |
| 1:B:304:PHE:N | 1:B:307:ALA:HB3 | 2.29 | 0.47 |
| 1:B:329:LYS:HA | 1:B:351:PRO:HA | 1.96 | 0.47 |
| 1:D:432:PRO:HA | 1:E:412:SER:HB3 | 1.97 | 0.47 |
| 1:G:94:ARG:NH1 | 1:G:103:GLU:OE2 | 2.46 | 0.47 |
| 1:G:315:LEU:HD12 | 1:G:339:VAL:CG2 | 2.45 | 0.47 |
| 1:I:208:ILE:O | 1:I:211:ARG:NH1 | 2.47 | 0.47 |
| 1:I:385:TRP:O | 1:I:389:LEU:HG | 2.15 | 0.47 |
| 1:J:95:TYR:OH | 1:J:145:THR:HG22 | 2.15 | 0.47 |
| 1:K:335:ASN:N | 1:K:335:ASN:OD1 | 2.47 | 0.47 |
| 1:A:387:LYS:O | 1:A:391:HIS:N | 2.47 | 0.46 |
| 1:B:219:VAL:HG13 | 1:B:373:LEU:HD21 | 1.97 | 0.46 |
| 1:C:315:LEU:HD11 | 1:C:335:ASN:HD22 | 1.79 | 0.46 |
| 1:G:40:GLN:HG2 | 1:G:43:ASN:HD21 | 1.78 | 0.46 |
| 1:G:85:HIS:CD2 | 1:G:86:ARG:HG2 | 2.49 | 0.46 |
| 1:G:117:VAL:HG23 | 1:G:485:ALA:HB2 | 1.97 | 0.46 |
| 1:G:331:LEU:HB2 | 1:G:352:THR:HA | 1.97 | 0.46 |
| 1:G:378:VAL:O | 1:G:382:TYR:N | 2.39 | 0.46 |
| 1:I:226:PHE:HE2 | 1:I:477:LEU:HD13 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:200:GLY:H | 1:K:384:GLU:CD | 2.23 | 0.46 |
| 1:K:321:ILE:HG12 | 1:K:343:ILE:HG23 | 1.96 | 0.46 |
| 1:L:287:ASP:OD1 | 1:L:287:ASP:N | 2.48 | 0.46 |
| 1:C:321:ILE:HA | 1:C:343:ILE:O | 2.15 | 0.46 |
| 1:G:116:ALA:HA | 2:G:601:XEG:OAC | 2.15 | 0.46 |
| 1:H:119:ASP:HA | 2:H:601:XEG:HAI | 1.96 | 0.46 |
| 1:C:343:ILE:HD11 | 1:C:368:ILE:HD11 | 1.96 | 0.46 |
| 1:E:79:ARG:NH2 | 1:E:163:ASP:OD2 | 2.36 | 0.46 |
| 1:E:96:SER:O | 1:E:130:LYS:HA | 2.15 | 0.46 |
| 1:F:189:HIS:C | 1:F:189:HIS:HD1 | 2.22 | 0.46 |
| 1:H:36:GLU:OE2 | 1:H:40:GLN:HB3 | 2.16 | 0.46 |
| 1:B:95:TYR:OH | 1:B:145:THR:HG22 | 2.16 | 0.46 |
| 1:C:10:PHE:O | 1:C:12:MET:N | 2.49 | 0.46 |
| 1:D:335:ASN:OD1 | 1:D:335:ASN:N | 2.48 | 0.46 |
| 1:D:446:LYS:HB3 | 1:D:450:HIS:HE1 | 1.80 | 0.46 |
| 1:J:323:ILE:HA | 1:J:345:ALA:O | 2.16 | 0.46 |
| 1:C:82:HIS:CG | 1:C:109:SER:HA | 2.51 | 0.46 |
| 1:C:458:GLU:OE1 | 1:D:400:LYS:NZ | 2.49 | 0.46 |
| 1:C:477:LEU:HD12 | 1:C:477:LEU:H | 1.81 | 0.46 |
| 1:E:99:VAL:O | 1:E:130:LYS:HE2 | 2.16 | 0.46 |
| 1:I:382:TYR:O | 1:I:386:LEU:HG | 2.15 | 0.46 |
| 1:L:65:ILE:HD13 | 1:L:144:ILE:HG12 | 1.97 | 0.46 |
| 1:L:238:MET:HG3 | 1:L:239:THR:H | 1.79 | 0.46 |
| 1:B:246:THR:HA | 1:B:269:LYS:O | 2.16 | 0.46 |
| 1:D:79:ARG:HA | 1:D:127:ALA:HA | 1.97 | 0.46 |
| 1:F:249:VAL:CG1 | 1:F:323:ILE:HD11 | 2.30 | 0.46 |
| 1:J:229:GLU:OE2 | 1:J:462:ARG:NH2 | 2.46 | 0.46 |
| 1:K:242:PHE:CE2 | 1:K:266:PHE:HB3 | 2.50 | 0.46 |
| 1:A:86:ARG:HH21 | 2:A:601:XEG:HBF | 1.81 | 0.46 |
| 1:A:245:LYS:HG2 | 1:A:320:ASP:OD2 | 2.15 | 0.46 |
| 1:B:17:PHE:O | 1:B:21:ALA:N | 2.32 | 0.46 |
| 1:B:150:MET:HG3 | 1:E:501:THR:CB | 2.46 | 0.46 |
| 1:B:294:PHE:CD2 | 1:B:301:ILE:HD12 | 2.51 | 0.46 |
| 1:B:456:THR:O | 1:B:460:SER:OG | 2.22 | 0.46 |
| 1:D:238:MET:HG2 | 1:D:245:LYS:HZ1 | 1.80 | 0.46 |
| 1:D:414:GLN:OE1 | 1:D:430:ILE:HG13 | 2.16 | 0.46 |
| 1:F:36:GLU:HG3 | 1:F:37:THR:H | 1.81 | 0.46 |
| 1:H:126:LYS:NZ | 1:H:168:ASP:OD2 | 2.45 | 0.46 |
| 1:I:60:SER:HB2 | 1:L:58:VAL:HG13 | 1.97 | 0.46 |
| 1:I:118:VAL:HG23 | 1:I:120:VAL:HG23 | 1.98 | 0.46 |
| 1:J:488:LYS:HE3 | 2:J:601:XEG:CAT | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:17:PHE:O | 1:L:21:ALA:N | 2.44 | 0.46 |
| 1:A:152:LEU:O | 1:A:157:PHE:N | 2.46 | 0.46 |
| 1:E:383:PHE:HA | 1:E:386:LEU:HD12 | 1.97 | 0.46 |
| 1:G:195:HIS:HD2 | 1:H:87:THR:HG21 | 1.80 | 0.46 |
| 1:H:332:THR:OG1 | 1:H:333:LYS:N | 2.47 | 0.46 |
| 1:H:436:PHE:O | 1:H:440:ILE:HG12 | 2.15 | 0.46 |
| 1:I:236:LEU:HD11 | 1:I:342:LYS:O | 2.16 | 0.46 |
| 1:J:42:ARG:HD3 | 1:J:46:ARG:HH21 | 1.81 | 0.46 |
| 1:L:87:THR:OG1 | 1:L:88:PRO:HD3 | 2.16 | 0.46 |
| 1:L:255:VAL:O | 1:L:259:SER:OG | 2.18 | 0.46 |
| 1:D:126:LYS:NZ | 1:D:168:ASP:OD2 | 2.46 | 0.46 |
| 1:D:206:GLY:O | 1:D:388:ASN:ND2 | 2.41 | 0.46 |
| 1:F:112:THR:OG1 | 1:F:124:GLY:HA3 | 2.15 | 0.46 |
| 1:F:242:PHE:CE2 | 1:F:266:PHE:HB3 | 2.44 | 0.46 |
| 1:H:294:PHE:HD2 | 1:H:301:ILE:HD12 | 1.80 | 0.46 |
| 1:H:311:GLU:HG3 | 1:H:312:GLY:N | 2.31 | 0.46 |
| 1:I:270:CYS:SG | 1:I:271:VAL:N | 2.87 | 0.46 |
| 2:I:601:XEG:HAJ | 2:I:601:XEG:HBE | 1.43 | 0.46 |
| 1:J:36:GLU:OE1 | 1:J:37:THR:N | 2.49 | 0.46 |
| 2:J:601:XEG:CAL | 2:J:601:XEG:HAP | 2.46 | 0.46 |
| 1:K:13:VAL:HG13 | 1:K:14:GLU:OE1 | 2.16 | 0.46 |
| 1:A:253:GLY:O | 1:A:255:VAL:N | 2.49 | 0.46 |
| 1:B:206:GLY:O | 1:B:388:ASN:ND2 | 2.39 | 0.46 |
| 1:B:305:PRO:C | 1:B:307:ALA:H | 2.24 | 0.46 |
| 1:B:315:LEU:HD12 | 1:B:339:VAL:CG2 | 2.46 | 0.46 |
| 1:D:324:PRO:HD2 | 1:D:345:ALA:O | 2.16 | 0.46 |
| 1:D:382:TYR:CE1 | 1:D:386:LEU:HD11 | 2.51 | 0.46 |
| 2:D:601:XEG:HAJ | 2:D:601:XEG:HBE | 1.43 | 0.46 |
| 1:G:480:ALA:O | 1:G:483:VAL:HG12 | 2.15 | 0.46 |
| 1:H:213:SER:HA | 1:H:258:HIS:ND1 | 2.31 | 0.46 |
| 1:I:193:ASN:ND2 | 1:I:389:LEU:HA | 2.30 | 0.46 |
| 1:I:226:PHE:C | 1:I:228:ASN:H | 2.24 | 0.46 |
| 1:I:346:GLU:HB3 | 1:I:370:ASP:HB3 | 1.98 | 0.46 |
| 1:K:136:TYR:HB2 | 1:K:141:LEU:CD1 | 2.46 | 0.46 |
| 1:K:226:PHE:HE2 | 1:K:477:LEU:CD1 | 2.29 | 0.46 |
| 1:K:432:PRO:HB2 | 1:K:436:PHE:HD1 | 1.80 | 0.46 |
| 1:A:330:GLN:O | 1:A:335:ASN:ND2 | 2.46 | 0.45 |
| 1:D:499:THR:HG22 | 1:D:501:THR:HG23 | 1.98 | 0.45 |
| 1:G:333:LYS:HG2 | 1:G:355:GLU:HG2 | 1.97 | 0.45 |
| 1:I:168:ASP:N | 1:I:171:THR:OG1 | 2.40 | 0.45 |
| 1:A:324:PRO:HD2 | 1:A:345:ALA:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:421:PHE:O | 1:B:423:LYS:N | 2.49 | 0.45 |
| 1:E:13:VAL:HA | 1:E:16:PHE:HD2 | 1.80 | 0.45 |
| 1:E:58:VAL:HG23 | 1:E:80:ALA:HB2 | 1.98 | 0.45 |
| 1:E:202:PRO:HG2 | 1:E:205:GLN:CG | 2.46 | 0.45 |
| 1:E:323:ILE:HA | 1:E:345:ALA:O | 2.16 | 0.45 |
| 1:F:193:ASN:OD1 | 1:F:193:ASN:N | 2.49 | 0.45 |
| 1:G:473:LEU:O | 1:G:475:LEU:N | 2.50 | 0.45 |
| 1:H:112:THR:OG1 | 1:H:124:GLY:HA3 | 2.17 | 0.45 |
| 1:J:462:ARG:HD2 | 1:J:466:ARG:HH21 | 1.81 | 0.45 |
| 1:L:236:LEU:HD11 | 1:L:342:LYS:O | 2.17 | 0.45 |
| 1:B:273:VAL:HG21 | 1:B:286:ILE:HD11 | 1.99 | 0.45 |
| 1:F:52:ILE:O | 1:F:82:HIS:NE2 | 2.50 | 0.45 |
| 1:G:315:LEU:HD12 | 1:G:339:VAL:HG22 | 1.96 | 0.45 |
| 1:H:257:LEU:HD11 | 1:H:295:LYS:HZ1 | 1.80 | 0.45 |
| 1:J:294:PHE:CD2 | 1:J:301:ILE:HG13 | 2.51 | 0.45 |
| 1:K:186:THR:OG1 | 1:K:187:ILE:N | 2.50 | 0.45 |
| 1:L:42:ARG:HD3 | 1:L:46:ARG:HH21 | 1.81 | 0.45 |
| 1:B:490:PHE:HE2 | 1:B:494:ASN:HD22 | 1.65 | 0.45 |
| 1:C:323:ILE:HG22 | 1:C:345:ALA:HB3 | 1.97 | 0.45 |
| 1:C:501:THR:CG2 | 1:F:150:MET:HG3 | 2.47 | 0.45 |
| 1:D:154:LYS:HB3 | 1:F:189:HIS:NE2 | 2.32 | 0.45 |
| 1:D:254:ASN:H | 1:D:257:LEU:HD12 | 1.81 | 0.45 |
| 1:E:499:THR:CG2 | 1:E:501:THR:HG23 | 2.46 | 0.45 |
| 1:G:9:PHE:HD1 | 1:G:10:PHE:H | 1.63 | 0.45 |
| 1:G:243:GLY:O | 1:G:245:LYS:N | 2.46 | 0.45 |
| 1:H:93:ILE:HD11 | 1:H:176:MET:HE1 | 1.97 | 0.45 |
| 1:I:112:THR:OG1 | 1:I:124:GLY:HA3 | 2.16 | 0.45 |
| 1:J:346:GLU:OE1 | 1:J:370:ASP:N | 2.44 | 0.45 |
| 1:K:207:GLY:O | 1:K:387:LYS:NZ | 2.35 | 0.45 |
| 1:K:281:TRP:CZ3 | 1:K:317:VAL:HG13 | 2.51 | 0.45 |
| 1:C:338:ARG:HG2 | 1:C:339:VAL:H | 1.81 | 0.45 |
| 1:K:126:LYS:HD2 | 1:K:126:LYS:HA | 1.84 | 0.45 |
| 1:L:226:PHE:C | 1:L:228:ASN:H | 2.25 | 0.45 |
| 1:A:208:ILE:H | 1:A:211:ARG:NH1 | 2.13 | 0.45 |
| 1:A:329:LYS:HB2 | 1:A:329:LYS:HE2 | 1.52 | 0.45 |
| 1:B:396:ARG:NE | 2:F:601:XEG:OAF | 2.47 | 0.45 |
| 1:I:87:THR:OG1 | 1:I:88:PRO:HD3 | 2.15 | 0.45 |
| 1:J:421:PHE:CZ | 1:J:423:LYS:HB3 | 2.51 | 0.45 |
| 1:C:38:GLU:O | 1:C:41:LYS:HD3 | 2.17 | 0.45 |
| 1:C:141:LEU:O | 1:C:145:THR:HG23 | 2.16 | 0.45 |
| 1:C:168:ASP:N | 1:C:171:THR:OG1 | 2.41 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:232:TYR:HB3 | 1:E:366:MET:HE1 | 1.99 | 0.45 |
| 1:E:251:GLY:HA3 | 1:E:326:ALA:HB2 | 1.97 | 0.45 |
| 1:E:345:ALA:HB1 | 1:E:373:LEU:HD22 | 1.98 | 0.45 |
| 1:F:86:ARG:HG2 | 1:F:121:PRO:C | 2.42 | 0.45 |
| 1:F:315:LEU:CD1 | 1:F:335:ASN:HD22 | 2.30 | 0.45 |
| 1:G:274:GLY:HA2 | 1:G:279:SER:HA | 1.97 | 0.45 |
| 1:H:232:TYR:HB3 | 1:H:366:MET:HE1 | 1.99 | 0.45 |
| 1:I:141:LEU:O | 1:I:145:THR:HG23 | 2.16 | 0.45 |
| 1:K:79:ARG:HA | 1:K:127:ALA:HA | 1.97 | 0.45 |
| 1:L:90:LYS:O | 1:L:125:ALA:N | 2.49 | 0.45 |
| 1:A:338:ARG:HG2 | 1:A:339:VAL:H | 1.81 | 0.45 |
| 1:E:95:TYR:OH | 1:E:145:THR:HG22 | 2.17 | 0.45 |
| 1:G:249:VAL:HA | 1:G:323:ILE:HG13 | 1.99 | 0.45 |
| 1:H:24:VAL:HG13 | 1:H:483:VAL:CG2 | 2.46 | 0.45 |
| 1:I:416:SER:HB3 | 1:K:429:PRO:HA | 1.99 | 0.45 |
| 1:J:480:ALA:HA | 1:J:483:VAL:HG11 | 1.98 | 0.45 |
| 1:L:46:ARG:HG2 | 1:L:50:ARG:HH11 | 1.82 | 0.45 |
| 1:L:211:ARG:HA | 1:L:214:ALA:HB2 | 1.98 | 0.45 |
| 1:D:249:VAL:HG12 | 1:D:323:ILE:CG1 | 2.47 | 0.45 |
| 1:F:86:ARG:HD2 | 1:F:86:ARG:HA | 1.84 | 0.45 |
| 1:F:118:VAL:HG23 | 1:F:120:VAL:HG23 | 1.97 | 0.45 |
| 1:F:202:PRO:HG2 | 1:F:205:GLN:HG3 | 1.99 | 0.45 |
| 1:G:90:LYS:HD2 | 1:G:164:VAL:O | 2.17 | 0.45 |
| 1:H:95:TYR:OH | 1:H:145:THR:HG22 | 2.16 | 0.45 |
| 1:I:200:GLY:HA2 | 1:I:211:ARG:HE | 1.81 | 0.45 |
| 1:J:249:VAL:CG2 | 1:J:273:VAL:HG22 | 2.46 | 0.45 |
| 1:B:330:GLN:O | 1:B:335:ASN:ND2 | 2.49 | 0.45 |
| 1:C:501:THR:HG22 | 1:F:150:MET:HG3 | 1.99 | 0.45 |
| 1:D:131:ILE:HB | 1:D:136:TYR:HE2 | 1.82 | 0.45 |
| 1:D:193:ASN:HD22 | 1:D:389:LEU:CD2 | 2.21 | 0.45 |
| 1:F:189:HIS:C | 1:F:189:HIS:ND1 | 2.75 | 0.45 |
| 1:G:197:CYS:SG | 1:G:198:VAL:HG12 | 2.57 | 0.45 |
| 1:I:79:ARG:HH11 | 1:I:127:ALA:HB2 | 1.81 | 0.45 |
| 1:I:95:TYR:HB3 | 1:I:133:PRO:HG3 | 1.98 | 0.45 |
| 1:J:167:PRO:HD3 | 1:J:176:MET:HG3 | 1.98 | 0.45 |
| 1:J:230:ALA:HA | 1:J:233:MET:HG2 | 1.98 | 0.45 |
| 1:J:304:PHE:H | 1:J:307:ALA:HB3 | 1.82 | 0.45 |
| 1:L:382:TYR:O | 1:L:386:LEU:HG | 2.17 | 0.45 |
| 1:A:244:ASP:O | 1:A:245:LYS:HG3 | 2.17 | 0.44 |
| 1:B:391:HIS:O | 1:F:382:TYR:OH | 2.34 | 0.44 |
| 1:E:247:PHE:HE1 | 1:E:260:MET:HG3 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:379:THR:O | 1:F:382:TYR:HB3 | 2.17 | 0.44 |
| 1:G:136:TYR:HB2 | 1:G:141:LEU:CD1 | 2.47 | 0.44 |
| 1:A:94:ARG:HE | 1:A:169:MET:CG | 2.31 | 0.44 |
| 1:B:72:TRP:HH2 | 1:E:498:VAL:HB | 1.81 | 0.44 |
| 1:B:86:ARG:HG3 | 1:B:121:PRO:HA | 1.98 | 0.44 |
| 1:B:193:ASN:OD1 | 1:B:193:ASN:N | 2.50 | 0.44 |
| 1:B:473:LEU:O | 1:B:475:LEU:N | 2.47 | 0.44 |
| 1:C:274:GLY:HA3 | 1:C:314:ILE:HD13 | 1.99 | 0.44 |
| 1:F:217:ARG:HA | 1:F:220:PHE:HB3 | 2.00 | 0.44 |
| 1:I:9:PHE:HB3 | 1:I:12:MET:CG | 2.43 | 0.44 |
| 1:F:315:LEU:HD22 | 1:F:322:LEU:HD21 | 1.98 | 0.44 |
| 2:H:601:XEG:CAZ | 2:H:601:XEG:HAP | 2.47 | 0.44 |
| 1:J:414:GLN:OE1 | 1:J:429:PRO:HD2 | 2.18 | 0.44 |
| 1:L:195:HIS:O | 1:L:201:LYS:HE3 | 2.18 | 0.44 |
| 1:C:324:PRO:HG2 | 1:C:351:PRO:HG2 | 1.99 | 0.44 |
| 1:G:21:ALA:HB1 | 1:G:49:LEU:HD23 | 1.99 | 0.44 |
| 1:G:250:GLN:HB2 | 1:G:324:PRO:HA | 2.00 | 0.44 |
| 2:J:601:XEG:HAP | 2:J:601:XEG:CAZ | 2.48 | 0.44 |
| 1:K:213:SER:HB3 | 1:K:262:TYR:HE2 | 1.83 | 0.44 |
| 1:K:253:GLY:O | 1:K:255:VAL:N | 2.51 | 0.44 |
| 1:K:473:LEU:O | 1:K:475:LEU:N | 2.50 | 0.44 |
| 1:L:175:GLU:O | 1:L:179:ILE:HG13 | 2.17 | 0.44 |
| 1:D:244:ASP:N | 1:D:244:ASP:OD1 | 2.46 | 0.44 |
| 1:E:463:GLN:OE1 | 1:E:488:LYS:NZ | 2.37 | 0.44 |
| 1:F:249:VAL:HA | 1:F:323:ILE:HG13 | 1.99 | 0.44 |
| 1:F:324:PRO:HG2 | 1:F:351:PRO:HG2 | 2.00 | 0.44 |
| 1:G:331:LEU:HD22 | 1:G:360:PHE:HZ | 1.82 | 0.44 |
| 2:G:601:XEG:HBE | 2:G:601:XEG:HAJ | 1.45 | 0.44 |
| 1:H:65:ILE:HD13 | 1:H:144:ILE:HG12 | 1.99 | 0.44 |
| 1:I:66:ARG:HD3 | 1:I:72:TRP:CE2 | 2.53 | 0.44 |
| 1:J:344:ILE:O | 1:J:367:VAL:HA | 2.18 | 0.44 |
| 1:K:42:ARG:O | 1:K:46:ARG:HG2 | 2.17 | 0.44 |
| 1:K:168:ASP:OD1 | 1:K:169:MET:N | 2.51 | 0.44 |
| 1:D:301:ILE:HG13 | 1:D:302:LEU:N | 2.31 | 0.44 |
| 1:D:322:LEU:O | 1:D:344:ILE:HA | 2.18 | 0.44 |
| 1:G:137:THR:H | 1:G:140:GLU:HB2 | 1.80 | 0.44 |
| 1:G:168:ASP:OD1 | 1:G:169:MET:HG2 | 2.17 | 0.44 |
| 1:G:358:LYS:HA | 1:G:361:LEU:CD2 | 2.48 | 0.44 |
| 1:I:323:ILE:HA | 1:I:345:ALA:O | 2.18 | 0.44 |
| 1:I:331:LEU:HB2 | 1:I:352:THR:HA | 1.99 | 0.44 |
| 1:K:226:PHE:C | 1:K:228:ASN:H | 2.25 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:244:ASP:N | 1:K:244:ASP:OD1 | 2.51 | 0.44 |
| 1:B:242:PHE:HE2 | 1:B:266:PHE:HB3 | 1.81 | 0.44 |
| 1:C:53:LYS:O | 1:C:82:HIS:HE1 | 2.00 | 0.44 |
| 2:E:601:XEG:HAJ | 2:E:601:XEG:HBE | 1.45 | 0.44 |
| 1:G:64:PRO:HB3 | 1:J:51:ILE:HG12 | 1.99 | 0.44 |
| 1:G:263:LEU:HD12 | 1:G:263:LEU:HA | 1.86 | 0.44 |
| 1:K:14:GLU:OE1 | 1:K:14:GLU:N | 2.51 | 0.44 |
| 1:L:421:PHE:CZ | 1:L:423:LYS:HB3 | 2.52 | 0.44 |
| 1:C:36:GLU:OE1 | 1:C:37:THR:N | 2.51 | 0.44 |
| 1:D:47:GLY:O | 1:D:51:ILE:HG13 | 2.18 | 0.44 |
| 1:E:165:PRO:HG2 | 1:E:198:VAL:HG23 | 1.99 | 0.44 |
| 1:I:336:ALA:HB3 | 1:I:359:ILE:HD12 | 2.00 | 0.44 |
| 1:J:79:ARG:NH2 | 1:J:163:ASP:OD2 | 2.37 | 0.44 |
| 1:C:432:PRO:HA | 1:D:412:SER:HB3 | 1.99 | 0.44 |
| 1:D:415:GLU:O | 1:D:419:ARG:HD2 | 2.18 | 0.44 |
| 1:E:387:LYS:O | 1:E:391:HIS:N | 2.51 | 0.44 |
| 1:F:445:GLU:O | 1:F:449:VAL:HG23 | 2.18 | 0.44 |
| 1:H:167:PRO:HD3 | 1:H:176:MET:HG3 | 2.00 | 0.44 |
| 1:J:209:HIS:HB3 | 1:J:446:LYS:HB3 | 2.00 | 0.44 |
| 1:J:495:GLU:OE1 | 1:K:204:SER:OG | 2.35 | 0.44 |
| 1:K:11:LYS:HB2 | 1:K:14:GLU:HG2 | 2.00 | 0.44 |
| 1:L:382:TYR:CZ | 1:L:386:LEU:HD11 | 2.53 | 0.44 |
| 1:A:499:THR:HG23 | 1:F:146:ARG:NH1 | 2.32 | 0.43 |
| 1:B:243:GLY:O | 1:B:245:LYS:N | 2.51 | 0.43 |
| 1:B:251:GLY:HA3 | 1:B:326:ALA:HB2 | 2.00 | 0.43 |
| 1:D:141:LEU:O | 1:D:145:THR:HG23 | 2.18 | 0.43 |
| 1:F:368:ILE:HG21 | 1:F:373:LEU:HD13 | 2.00 | 0.43 |
| 1:G:281:TRP:CZ3 | 1:G:317:VAL:HG13 | 2.53 | 0.43 |
| 1:H:383:PHE:HA | 1:H:386:LEU:HD12 | 2.00 | 0.43 |
| 1:I:142:GLU:HG3 | 1:I:178:TRP:CD2 | 2.53 | 0.43 |
| 1:J:238:MET:HE3 | 1:J:342:LYS:HD2 | 2.00 | 0.43 |
| 2:J:601:XEG:HAJ | 2:J:601:XEG:HBE | 1.48 | 0.43 |
| 1:K:11:LYS:HB2 | 1:K:14:GLU:CG | 2.48 | 0.43 |
| 1:K:294:PHE:HE2 | 1:K:302:LEU:H | 1.65 | 0.43 |
| 1:A:24:VAL:HG13 | 1:A:483:VAL:HG23 | 1.99 | 0.43 |
| 1:B:281:TRP:CZ3 | 1:B:317:VAL:HG13 | 2.53 | 0.43 |
| 1:C:61:LEU:HD21 | 1:C:151:GLU:CB | 2.48 | 0.43 |
| 1:C:387:LYS:HD2 | 1:C:445:GLU:OE2 | 2.17 | 0.43 |
| 1:D:36:GLU:HG2 | 1:D:38:GLU:OE2 | 2.18 | 0.43 |
| 1:I:89:CYS:HB3 | 1:I:125:ALA:HB2 | 2.00 | 0.43 |
| 1:I:137:THR:H | 1:I:140:GLU:HB2 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:454:ALA:O | 1:A:457:MET:N | 2.51 | 0.43 |
| 1:B:332:THR:OG1 | 1:B:333:LYS:N | 2.52 | 0.43 |
| 2:D:601:XEG:OAF | 1:E:396:ARG:NE | 2.50 | 0.43 |
| 1:F:193:ASN:HD22 | 1:F:389:LEU:HA | 1.83 | 0.43 |
| 1:H:24:VAL:HG13 | 1:H:483:VAL:HG22 | 2.00 | 0.43 |
| 1:I:99:VAL:O | 1:I:130:LYS:HE2 | 2.18 | 0.43 |
| 1:I:102:ASP:HA | 1:I:105:LYS:HB3 | 2.00 | 0.43 |
| 1:I:346:GLU:CD | 1:I:478:ARG:HH12 | 2.25 | 0.43 |
| 1:L:236:LEU:HD21 | 1:L:342:LYS:HB3 | 2.00 | 0.43 |
| 1:L:238:MET:HG3 | 1:L:239:THR:N | 2.32 | 0.43 |
| 1:C:36:GLU:OE1 | 1:C:41:LYS:HG3 | 2.18 | 0.43 |
| 1:E:304:PHE:N | 1:E:307:ALA:HB3 | 2.32 | 0.43 |
| 1:F:14:GLU:OE1 | 1:F:14:GLU:N | 2.45 | 0.43 |
| 1:F:207:GLY:HA3 | 1:F:211:ARG:NH1 | 2.33 | 0.43 |
| 1:H:88:PRO:HG2 | 1:H:122:PHE:CD2 | 2.54 | 0.43 |
| 1:I:258:HIS:HA | 1:I:261:ARG:HB3 | 1.99 | 0.43 |
| 1:J:90:LYS:HE3 | 1:J:378:VAL:HG23 | 2.00 | 0.43 |
| 1:J:253:GLY:O | 1:J:255:VAL:N | 2.51 | 0.43 |
| 1:J:324:PRO:HD2 | 1:J:345:ALA:O | 2.17 | 0.43 |
| 1:A:148:PHE:CZ | 1:A:152:LEU:HD11 | 2.54 | 0.43 |
| 1:A:416:SER:HB3 | 1:B:429:PRO:HA | 2.01 | 0.43 |
| 1:B:301:ILE:HG13 | 1:B:302:LEU:N | 2.34 | 0.43 |
| 1:D:193:ASN:OD1 | 1:D:193:ASN:N | 2.52 | 0.43 |
| 1:D:427:THR:HG22 | 1:D:429:PRO:HD3 | 2.01 | 0.43 |
| 1:E:414:GLN:OE1 | 1:E:429:PRO:HD2 | 2.17 | 0.43 |
| 1:H:145:THR:O | 1:H:149:THR:OG1 | 2.36 | 0.43 |
| 1:H:211:ARG:HA | 1:H:214:ALA:HB2 | 1.99 | 0.43 |
| 1:H:432:PRO:HB2 | 1:H:436:PHE:HD1 | 1.84 | 0.43 |
| 1:K:257:LEU:HB3 | 1:K:258:HIS:HD2 | 1.83 | 0.43 |
| 1:K:480:ALA:O | 1:K:483:VAL:HG12 | 2.18 | 0.43 |
| 1:K:494:ASN:HD22 | 1:K:494:ASN:C | 2.25 | 0.43 |
| 1:A:52:ILE:HG12 | 1:A:493:TYR:HE2 | 1.84 | 0.43 |
| 1:B:36:GLU:HG3 | 1:B:37:THR:N | 2.32 | 0.43 |
| 1:C:478:ARG:HD2 | 1:C:482:TYR:HE2 | 1.84 | 0.43 |
| 1:E:207:GLY:HA2 | 1:E:384:GLU:OE1 | 2.18 | 0.43 |
| 1:E:254:ASN:N | 1:E:257:LEU:HD12 | 2.33 | 0.43 |
| 1:F:91:GLY:O | 1:F:165:PRO:HA | 2.18 | 0.43 |
| 1:F:257:LEU:HD11 | 1:F:295:LYS:CE | 2.49 | 0.43 |
| 1:I:352:THR:HG23 | 1:I:360:PHE:HE2 | 1.84 | 0.43 |
| 1:L:227:ILE:HG23 | 1:L:233:MET:HE3 | 2.00 | 0.43 |
| 1:L:263:LEU:HD12 | 1:L:263:LEU:HA | 1.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:295:LYS:HB3 | 1:B:296:LEU:H | 1.53 | 0.43 |
| 1:B:477:LEU:O | 1:B:481:ALA:N | 2.52 | 0.43 |
| 1:F:263:LEU:HD12 | 1:F:263:LEU:HA | 1.70 | 0.43 |
| 1:F:287:ASP:CG | 1:F:289:LYS:HD3 | 2.44 | 0.43 |
| 1:G:477:LEU:HD12 | 1:G:477:LEU:H | 1.82 | 0.43 |
| 1:I:224:GLU:C | 1:I:226:PHE:H | 2.27 | 0.43 |
| 1:I:446:LYS:HG2 | 1:I:450:HIS:CD2 | 2.54 | 0.43 |
| 1:J:215:THR:O | 1:J:219:VAL:HG23 | 2.18 | 0.43 |
| 1:K:52:ILE:O | 1:K:82:HIS:NE2 | 2.51 | 0.43 |
| 1:K:90:LYS:HD2 | 1:K:164:VAL:O | 2.19 | 0.43 |
| 1:L:90:LYS:NZ | 1:L:381:SER:HB3 | 2.34 | 0.43 |
| 1:A:414:GLN:OE1 | 1:A:430:ILE:HG23 | 2.18 | 0.43 |
| 1:D:48:ILE:O | 1:D:52:ILE:HG13 | 2.18 | 0.43 |
| 1:D:446:LYS:HB3 | 1:D:450:HIS:CE1 | 2.53 | 0.43 |
| 1:E:193:ASN:HD22 | 1:E:389:LEU:HA | 1.82 | 0.43 |
| 1:H:226:PHE:C | 1:H:228:ASN:H | 2.27 | 0.43 |
| 1:J:86:ARG:HA | 1:J:86:ARG:HD3 | 1.83 | 0.43 |
| 1:A:152:LEU:HB3 | 1:A:157:PHE:HB2 | 2.00 | 0.43 |
| 1:A:328:GLU:CD | 1:A:329:LYS:HZ2 | 2.27 | 0.43 |
| 1:B:12:MET:HE3 | 1:B:12:MET:HB2 | 1.79 | 0.43 |
| 2:C:601:XEG:HBE | 2:C:601:XEG:HAJ | 1.44 | 0.43 |
| 1:D:215:THR:O | 1:D:219:VAL:HG23 | 2.18 | 0.43 |
| 1:D:348:ALA:HB3 | 1:D:351:PRO:HG3 | 2.01 | 0.43 |
| 1:E:368:ILE:HA | 1:E:369:PRO:HD3 | 1.89 | 0.43 |
| 1:G:12:MET:SD | 1:G:329:LYS:HE2 | 2.59 | 0.43 |
| 1:G:19:ARG:HD3 | 1:G:479:THR:HG21 | 2.01 | 0.43 |
| 1:I:321:ILE:HG12 | 1:I:343:ILE:CG2 | 2.49 | 0.43 |
| 1:J:207:GLY:HA2 | 1:J:384:GLU:OE1 | 2.19 | 0.43 |
| 1:J:247:PHE:HA | 1:J:319:CYS:SG | 2.59 | 0.43 |
| 1:J:436:PHE:O | 1:J:440:ILE:HG12 | 2.18 | 0.43 |
| 1:L:280:ILE:HD11 | 1:L:301:ILE:HD11 | 2.01 | 0.43 |
| 1:L:282:ASN:HD21 | 1:L:306:LYS:CG | 2.18 | 0.43 |
| 1:A:36:GLU:CG | 1:A:38:GLU:CG | 2.94 | 0.43 |
| 1:C:249:VAL:HG12 | 1:C:323:ILE:CD1 | 2.43 | 0.43 |
| 1:C:392:VAL:HG13 | 1:E:386:LEU:HD22 | 2.01 | 0.43 |
| 1:F:95:TYR:OH | 1:F:145:THR:HG22 | 2.19 | 0.43 |
| 1:H:10:PHE:O | 1:H:12:MET:N | 2.42 | 0.43 |
| 1:K:219:VAL:HG13 | 1:K:373:LEU:HD21 | 2.01 | 0.43 |
| 1:K:414:GLN:OE1 | 1:K:430:ILE:HG23 | 2.19 | 0.43 |
| 1:L:19:ARG:HE | 1:L:479:THR:HG21 | 1.82 | 0.43 |
| 1:A:6:ASP:HA | 1:A:7:PRO:HD3 | 1.93 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:246:THR:HB | 1:A:271:VAL:HB | 2.00 | 0.42 |
| 1:C:120:VAL:O | 1:C:122:PHE:N | 2.46 | 0.42 |
| 1:C:131:ILE:HB | 1:C:136:TYR:CE2 | 2.52 | 0.42 |
| 1:C:246:THR:HA | 1:C:269:LYS:O | 2.19 | 0.42 |
| 1:C:423:LYS:HE3 | 1:C:423:LYS:HB3 | 1.73 | 0.42 |
| 1:D:202:PRO:HA | 1:D:211:ARG:HH22 | 1.84 | 0.42 |
| 1:E:24:VAL:HG13 | 1:E:483:VAL:HG22 | 2.00 | 0.42 |
| 1:F:46:ARG:HB3 | 1:F:50:ARG:HH11 | 1.83 | 0.42 |
| 1:G:61:LEU:HD21 | 1:G:151:GLU:HB2 | 2.01 | 0.42 |
| 1:G:313:SER:OG | 1:G:314:ILE:N | 2.49 | 0.42 |
| 1:G:414:GLN:OE1 | 1:G:429:PRO:HD2 | 2.19 | 0.42 |
| 1:H:255:VAL:HG13 | 1:H:256:GLY:H | 1.84 | 0.42 |
| 1:K:14:GLU:H | 1:K:14:GLU:CD | 2.27 | 0.42 |
| 1:L:131:ILE:HB | 1:L:136:TYR:HE2 | 1.84 | 0.42 |
| 2:L:601:XEG:CAL | 2:L:601:XEG:HAP | 2.49 | 0.42 |
| 1:A:27:LYS:HB2 | 1:A:27:LYS:HE3 | 1.74 | 0.42 |
| 1:A:168:ASP:OD1 | 1:A:169:MET:N | 2.52 | 0.42 |
| 1:A:331:LEU:HB2 | 1:A:352:THR:HA | 2.01 | 0.42 |
| 1:B:67:ARG:NH2 | 1:B:135:ASN:O | 2.52 | 0.42 |
| 1:B:345:ALA:HA | 1:B:368:ILE:HB | 2.01 | 0.42 |
| 1:C:294:PHE:HD2 | 1:C:301:ILE:HD12 | 1.80 | 0.42 |
| 1:D:305:PRO:C | 1:D:307:ALA:H | 2.27 | 0.42 |
| 1:E:36:GLU:HB3 | 1:E:37:THR:H | 1.68 | 0.42 |
| 1:E:416:SER:O | 1:E:419:ARG:HB2 | 2.19 | 0.42 |
| 1:F:166:ALA:HB1 | 1:F:167:PRO:HD2 | 2.00 | 0.42 |
| 1:J:6:ASP:HA | 1:J:7:PRO:HD3 | 1.90 | 0.42 |
| 1:J:159:GLY:N | 1:J:163:ASP:O | 2.47 | 0.42 |
| 1:J:417:LEU:C | 1:J:419:ARG:H | 2.27 | 0.42 |
| 1:L:321:ILE:HG12 | 1:L:343:ILE:CG2 | 2.49 | 0.42 |
| 1:B:482:TYR:O | 1:B:486:ILE:HG13 | 2.19 | 0.42 |
| 1:D:217:ARG:HD3 | 1:D:262:TYR:CE2 | 2.54 | 0.42 |
| 1:D:371:LEU:HD23 | 1:D:481:ALA:HB1 | 2.01 | 0.42 |
| 1:E:462:ARG:HD3 | 1:E:465:MET:HE2 | 2.00 | 0.42 |
| 1:G:217:ARG:NE | 1:G:450:HIS:HD2 | 2.16 | 0.42 |
| 1:G:488:LYS:O | 1:G:492:VAL:HG23 | 2.18 | 0.42 |
| 1:I:232:TYR:HD1 | 1:I:235:ILE:HD12 | 1.84 | 0.42 |
| 1:K:107:LEU:HB3 | 1:K:126:LYS:HG2 | 2.00 | 0.42 |
| 1:K:421:PHE:CZ | 1:K:423:LYS:HE3 | 2.53 | 0.42 |
| 1:A:251:GLY:HA3 | 1:A:326:ALA:HB2 | 2.02 | 0.42 |
| 1:A:432:PRO:HB2 | 1:A:436:PHE:HD1 | 1.84 | 0.42 |
| 1:C:336:ALA:C | 1:C:338:ARG:H | 2.27 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:27:LYS:HB2 | 1:E:27:LYS:HE2 | 1.81 | 0.42 |
| 1:E:329:LYS:HA | 1:E:351:PRO:O | 2.19 | 0.42 |
| 1:F:382:TYR:CZ | 1:F:386:LEU:HD11 | 2.54 | 0.42 |
| 1:G:126:LYS:HD2 | 1:G:126:LYS:HA | 1.87 | 0.42 |
| 1:H:118:VAL:HA | 1:H:460:SER:OG | 2.19 | 0.42 |
| 1:H:227:ILE:HA | 1:H:233:MET:CE | 2.48 | 0.42 |
| 1:H:378:VAL:O | 1:H:382:TYR:N | 2.48 | 0.42 |
| 1:H:498:VAL:HG13 | 1:H:498:VAL:O | 2.19 | 0.42 |
| 1:A:275:GLU:HB3 | 1:A:276:SER:H | 1.55 | 0.42 |
| 1:B:350:GLY:N | 1:B:370:ASP:OD2 | 2.50 | 0.42 |
| 2:C:601:XEG:CAZ | 2:C:601:XEG:HAP | 2.50 | 0.42 |
| 1:D:32:LEU:HG | 1:D:34:THR:HG22 | 2.00 | 0.42 |
| 1:G:491:ARG:H | 1:G:491:ARG:HG2 | 1.50 | 0.42 |
| 1:G:495:GLU:O | 1:L:177:SER:OG | 2.28 | 0.42 |
| 1:H:52:ILE:HD13 | 1:H:489:VAL:HG12 | 2.02 | 0.42 |
| 1:I:271:VAL:HG23 | 1:I:283:PRO:HA | 2.02 | 0.42 |
| 1:L:91:GLY:O | 1:L:165:PRO:HA | 2.20 | 0.42 |
| 1:A:97:THR:N | 1:A:131:ILE:O | 2.53 | 0.42 |
| 1:C:86:ARG:HD3 | 1:C:86:ARG:HA | 1.92 | 0.42 |
| 1:C:193:ASN:OD1 | 1:C:193:ASN:N | 2.52 | 0.42 |
| 1:E:201:LYS:HE2 | 1:E:206:GLY:O | 2.20 | 0.42 |
| 1:E:263:LEU:HA | 1:E:263:LEU:HD12 | 1.78 | 0.42 |
| 1:E:382:TYR:CE1 | 1:E:386:LEU:HD11 | 2.55 | 0.42 |
| 1:E:394:TYR:N | 1:E:445:GLU:HG3 | 2.34 | 0.42 |
| 2:F:601:XEG:CAL | 2:F:601:XEG:HAP | 2.49 | 0.42 |
| 1:H:141:LEU:O | 1:H:145:THR:HG23 | 2.18 | 0.42 |
| 1:J:168:ASP:OD1 | 1:J:169:MET:N | 2.52 | 0.42 |
| 1:J:333:LYS:NZ | 1:J:355:GLU:HG2 | 2.34 | 0.42 |
| 1:L:315:LEU:HD11 | 1:L:335:ASN:HB2 | 2.01 | 0.42 |
| 1:A:90:LYS:HE2 | 1:A:378:VAL:HG23 | 2.01 | 0.42 |
| 1:D:331:LEU:HA | 1:D:335:ASN:ND2 | 2.33 | 0.42 |
| 1:F:287:ASP:OD1 | 1:F:289:LYS:HD3 | 2.19 | 0.42 |
| 1:F:433:THR:HG23 | 1:F:436:PHE:H | 1.85 | 0.42 |
| 1:G:488:LYS:HG2 | 2:G:601:XEG:CAN | 2.50 | 0.42 |
| 1:H:208:ILE:HG22 | 1:H:211:ARG:HD3 | 2.00 | 0.42 |
| 1:I:90:LYS:NZ | 1:I:381:SER:HB3 | 2.35 | 0.42 |
| 1:K:52:ILE:HG12 | 1:K:493:TYR:CE2 | 2.55 | 0.42 |
| 1:L:90:LYS:HD2 | 1:L:164:VAL:O | 2.20 | 0.42 |
| 1:L:223:ILE:O | 1:L:227:ILE:HG12 | 2.19 | 0.42 |
| 1:L:370:ASP:OD1 | 1:L:370:ASP:N | 2.52 | 0.42 |
| 2:L:601:XEG:HBE | 2:L:601:XEG:HAJ | 1.46 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:316:GLU:HA | 1:A:339:VAL:HA | 2.01 | 0.42 |
| 1:D:80:ALA:O | 1:D:125:ALA:HA | 2.20 | 0.42 |
| 1:D:304:PHE:N | 1:D:307:ALA:HB3 | 2.34 | 0.42 |
| 1:E:14:GLU:OE1 | 1:E:14:GLU:N | 2.44 | 0.42 |
| 1:K:85:HIS:CD2 | 1:K:86:ARG:HG2 | 2.54 | 0.42 |
| 1:K:129:VAL:HG12 | 1:K:131:ILE:HG12 | 2.00 | 0.42 |
| 1:L:9:PHE:CD2 | 1:L:12:MET:HG2 | 2.54 | 0.42 |
| 1:L:95:TYR:OH | 1:L:145:THR:HG22 | 2.20 | 0.42 |
| 1:C:143:LYS:O | 1:C:147:ARG:HB2 | 2.20 | 0.42 |
| 1:C:146:ARG:HG2 | 1:C:182:THR:OG1 | 2.19 | 0.42 |
| 1:F:414:GLN:OE1 | 1:F:429:PRO:HD2 | 2.20 | 0.42 |
| 1:H:257:LEU:HD11 | 1:H:295:LYS:NZ | 2.35 | 0.42 |
| 1:I:145:THR:OG1 | 1:I:146:ARG:N | 2.52 | 0.42 |
| 1:I:201:LYS:HE2 | 1:I:206:GLY:O | 2.20 | 0.42 |
| 1:L:465:MET:O | 1:L:469:MET:HG3 | 2.20 | 0.42 |
| 1:A:350:GLY:N | 1:A:351:PRO:HD3 | 2.35 | 0.42 |
| 1:D:129:VAL:HG12 | 1:D:131:ILE:HG12 | 2.01 | 0.42 |
| 1:F:41:LYS:H | 1:F:41:LYS:HG3 | 1.58 | 0.42 |
| 1:G:165:PRO:HD2 | 1:G:197:CYS:O | 2.19 | 0.42 |
| 1:H:10:PHE:O | 1:H:12:MET:HG3 | 2.19 | 0.42 |
| 1:J:65:ILE:HD13 | 1:J:144:ILE:HG12 | 2.01 | 0.42 |
| 1:J:324:PRO:HG2 | 1:J:351:PRO:HG2 | 2.01 | 0.42 |
| 1:J:382:TYR:CE2 | 1:J:386:LEU:HD11 | 2.55 | 0.42 |
| 1:K:243:GLY:O | 1:K:245:LYS:N | 2.44 | 0.42 |
| 1:A:7:PRO:HB2 | 1:A:8:ASN:H | 1.69 | 0.41 |
| 1:A:94:ARG:HG2 | 1:A:169:MET:HB2 | 2.02 | 0.41 |
| 1:A:167:PRO:HD3 | 1:A:176:MET:HG3 | 2.02 | 0.41 |
| 1:B:160:PRO:HG3 | 1:B:193:ASN:O | 2.19 | 0.41 |
| 1:C:213:SER:CB | 1:C:262:TYR:HE2 | 2.33 | 0.41 |
| 1:C:379:THR:O | 1:C:382:TYR:HB3 | 2.20 | 0.41 |
| 1:E:201:LYS:HD2 | 1:E:205:GLN:O | 2.20 | 0.41 |
| 1:G:16:PHE:CZ | 1:G:354:PRO:HD3 | 2.55 | 0.41 |
| 1:G:260:MET:HE1 | 1:G:286:ILE:HD11 | 2.01 | 0.41 |
| 1:G:271:VAL:HG23 | 1:G:283:PRO:HA | 2.02 | 0.41 |
| 1:H:158:ILE:HD12 | 1:H:165:PRO:CD | 2.50 | 0.41 |
| 1:H:491:ARG:H | 1:H:491:ARG:HG2 | 1.62 | 0.41 |
| 1:J:371:LEU:HD23 | 1:J:481:ALA:HB1 | 2.02 | 0.41 |
| 1:K:217:ARG:HH11 | 1:K:217:ARG:HD3 | 1.68 | 0.41 |
| 1:L:242:PHE:CE2 | 1:L:266:PHE:HB3 | 2.53 | 0.41 |
| 1:A:37:THR:O | 1:A:37:THR:OG1 | 2.32 | 0.41 |
| 1:A:368:ILE:HA | 1:A:369:PRO:HD3 | 1.95 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:494:ASN:C | 1:A:494:ASN:HD22 | 2.28 | 0.41 |
| 1:C:148:PHE:O | 1:C:152:LEU:HG | 2.19 | 0.41 |
| 1:C:215:THR:O | 1:C:219:VAL:HG23 | 2.20 | 0.41 |
| 2:C:601:XEG:HAP | 2:C:601:XEG:CAL | 2.50 | 0.41 |
| 1:D:107:LEU:HD23 | 1:D:126:LYS:HE2 | 2.02 | 0.41 |
| 1:D:112:THR:OG1 | 1:D:124:GLY:HA3 | 2.20 | 0.41 |
| 1:E:66:ARG:HD2 | 1:E:70:GLY:HA2 | 2.01 | 0.41 |
| 1:E:433:THR:HG23 | 1:E:436:PHE:H | 1.84 | 0.41 |
| 1:F:346:GLU:HG2 | 1:F:351:PRO:HD2 | 2.02 | 0.41 |
| 1:G:164:VAL:HG13 | 1:G:198:VAL:HA | 2.02 | 0.41 |
| 1:G:215:THR:O | 1:G:219:VAL:HG23 | 2.21 | 0.41 |
| 1:G:244:ASP:O | 1:G:245:LYS:HD2 | 2.20 | 0.41 |
| 1:I:429:PRO:HA | 1:J:416:SER:HB3 | 2.02 | 0.41 |
| 1:K:58:VAL:HA | 1:K:80:ALA:HA | 2.02 | 0.41 |
| 1:K:378:VAL:HA | 1:K:381:SER:HB2 | 2.01 | 0.41 |
| 1:A:93:ILE:HD11 | 1:A:176:MET:HE1 | 2.01 | 0.41 |
| 1:B:315:LEU:HD11 | 1:B:335:ASN:HB2 | 2.02 | 0.41 |
| 1:B:324:PRO:HD2 | 1:B:345:ALA:O | 2.20 | 0.41 |
| 1:D:88:PRO:HG2 | 1:D:122:PHE:CE2 | 2.55 | 0.41 |
| 1:D:131:ILE:HB | 1:D:136:TYR:CE2 | 2.55 | 0.41 |
| 1:D:250:GLN:HB2 | 1:D:314:ILE:HG21 | 2.02 | 0.41 |
| 1:E:248:ALA:CB | 1:E:272:ALA:HB3 | 2.50 | 0.41 |
| 1:E:253:GLY:HA2 | 1:E:295:LYS:HZ1 | 1.86 | 0.41 |
| 1:E:454:ALA:O | 1:E:457:MET:N | 2.53 | 0.41 |
| 1:G:129:VAL:HG12 | 1:G:131:ILE:HG12 | 2.02 | 0.41 |
| 1:H:46:ARG:HG2 | 1:H:50:ARG:HH11 | 1.84 | 0.41 |
| 1:I:195:HIS:CE1 | 1:K:87:THR:HG22 | 2.54 | 0.41 |
| 1:I:445:GLU:O | 1:I:449:VAL:HG23 | 2.20 | 0.41 |
| 1:J:19:ARG:HG2 | 1:J:479:THR:HG22 | 2.02 | 0.41 |
| 1:K:164:VAL:HG13 | 1:K:198:VAL:HA | 2.01 | 0.41 |
| 1:K:327:SER:OG | 1:K:328:GLU:N | 2.53 | 0.41 |
| 1:K:336:ALA:N | 1:K:337:PRO:HD2 | 2.35 | 0.41 |
| 1:A:214:ALA:HB1 | 1:A:377:GLY:HA2 | 2.03 | 0.41 |
| 1:E:131:ILE:HB | 1:E:136:TYR:HE2 | 1.85 | 0.41 |
| 1:E:324:PRO:HD2 | 1:E:345:ALA:O | 2.19 | 0.41 |
| 1:E:432:PRO:HB2 | 1:E:436:PHE:HD1 | 1.85 | 0.41 |
| 1:G:300:THR:CG2 | 1:G:301:ILE:H | 2.33 | 0.41 |
| 1:H:14:GLU:H | 1:H:14:GLU:HG2 | 1.66 | 0.41 |
| 1:K:371:LEU:HD23 | 1:K:481:ALA:HB1 | 2.01 | 0.41 |
| 1:K:409:LEU:O | 1:K:412:SER:N | 2.54 | 0.41 |
| 1:L:323:ILE:HA | 1:L:345:ALA:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:193:ASN:ND2 | 1:B:389:LEU:HD22 | 2.29 | 0.41 |
| 1:B:371:LEU:HD23 | 1:B:481:ALA:HB1 | 2.02 | 0.41 |
| 1:C:294:PHE:HE2 | 1:C:302:LEU:H | 1.67 | 0.41 |
| 1:D:9:PHE:HE1 | 1:D:329:LYS:NZ | 2.18 | 0.41 |
| 1:E:24:VAL:HG13 | 1:E:483:VAL:CG2 | 2.50 | 0.41 |
| 1:E:34:THR:OG1 | 1:E:35:ARG:N | 2.53 | 0.41 |
| 1:F:91:GLY:HA3 | 1:F:125:ALA:O | 2.21 | 0.41 |
| 1:G:244:ASP:OD1 | 1:G:244:ASP:N | 2.51 | 0.41 |
| 1:H:270:CYS:SG | 1:H:271:VAL:N | 2.94 | 0.41 |
| 1:I:263:LEU:HD12 | 1:I:263:LEU:HA | 1.89 | 0.41 |
| 1:K:294:PHE:CZ | 1:K:304:PHE:CE1 | 3.09 | 0.41 |
| 1:L:332:THR:HA | 1:L:356:ALA:HB2 | 2.01 | 0.41 |
| 1:A:86:ARG:HD3 | 1:A:86:ARG:HA | 1.91 | 0.41 |
| 1:B:42:ARG:HD3 | 1:B:46:ARG:HH21 | 1.86 | 0.41 |
| 1:C:136:TYR:HB2 | 1:C:141:LEU:HD13 | 2.02 | 0.41 |
| 1:E:253:GLY:O | 1:E:255:VAL:N | 2.54 | 0.41 |
| 1:F:134:LYS:H | 1:F:134:LYS:HG2 | 1.57 | 0.41 |
| 1:G:50:ARG:O | 1:J:74:VAL:HG11 | 2.21 | 0.41 |
| 1:G:421:PHE:HZ | 1:G:423:LYS:HE2 | 1.86 | 0.41 |
| 1:G:432:PRO:HB2 | 1:G:436:PHE:HD1 | 1.86 | 0.41 |
| 1:H:207:GLY:HA2 | 1:H:384:GLU:OE1 | 2.20 | 0.41 |
| 1:J:36:GLU:OE1 | 1:J:41:LYS:HG2 | 2.21 | 0.41 |
| 1:L:42:ARG:O | 1:L:46:ARG:N | 2.35 | 0.41 |
| 1:L:305:PRO:C | 1:L:307:ALA:H | 2.29 | 0.41 |
| 1:B:79:ARG:HA | 1:B:127:ALA:HA | 2.02 | 0.41 |
| 1:B:500:PHE:HB3 | 1:D:500:PHE:HB3 | 2.03 | 0.41 |
| 1:C:321:ILE:HG12 | 1:C:343:ILE:HG23 | 2.03 | 0.41 |
| 1:E:461:ALA:O | 1:E:465:MET:HG3 | 2.20 | 0.41 |
| 1:F:383:PHE:HA | 1:F:386:LEU:HD12 | 2.03 | 0.41 |
| 1:H:32:LEU:HD13 | 1:H:494:ASN:HD21 | 1.85 | 0.41 |
| 1:H:47:GLY:HA3 | 1:K:72:TRP:HB2 | 2.03 | 0.41 |
| 1:H:345:ALA:HB1 | 1:H:373:LEU:HD22 | 2.02 | 0.41 |
| 1:J:28:LEU:HD22 | 1:J:490:PHE:CD2 | 2.56 | 0.41 |
| 1:J:61:LEU:HD12 | 1:J:61:LEU:HA | 1.87 | 0.41 |
| 1:J:212:ILE:HG13 | 1:J:258:HIS:CE1 | 2.45 | 0.41 |
| 1:J:376:GLY:HA2 | 1:J:379:THR:HB | 2.03 | 0.41 |
| 1:L:459:ARG:O | 1:L:463:GLN:HG3 | 2.20 | 0.41 |
| 1:B:48:ILE:O | 1:B:52:ILE:HG13 | 2.20 | 0.41 |
| 1:C:249:VAL:HA | 1:C:323:ILE:HG13 | 2.02 | 0.41 |
| 1:D:134:LYS:H | 1:D:134:LYS:HG2 | 1.47 | 0.41 |
| 1:E:229:GLU:OE2 | 1:E:462:ARG:NH2 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:327:SER:OG | 1:E:328:GLU:N | 2.54 | 0.41 |
| 1:E:350:GLY:N | 1:E:351:PRO:HD3 | 2.35 | 0.41 |
| 1:H:408:HIS:HB3 | 1:L:436:PHE:CD2 | 2.56 | 0.41 |
| 1:J:227:ILE:HD12 | 1:J:242:PHE:CD1 | 2.53 | 0.41 |
| 1:L:29:VAL:O | 1:L:41:LYS:NZ | 2.53 | 0.41 |
| 1:L:79:ARG:HH11 | 1:L:127:ALA:HB2 | 1.85 | 0.41 |
| 1:L:201:LYS:HG2 | 1:L:384:GLU:OE1 | 2.21 | 0.41 |
| 1:A:12:MET:HG3 | 1:A:13:VAL:H | 1.86 | 0.41 |
| 1:A:183:TYR:CE2 | 1:A:188:GLY:HA3 | 2.56 | 0.41 |
| 1:A:193:ASN:OD1 | 1:A:193:ASN:N | 2.54 | 0.41 |
| 1:A:211:ARG:HA | 1:A:380:VAL:HG11 | 2.02 | 0.41 |
| 1:A:323:ILE:HA | 1:A:345:ALA:O | 2.21 | 0.41 |
| 1:B:219:VAL:HA | 1:B:373:LEU:HG | 2.02 | 0.41 |
| 1:D:186:THR:OG1 | 1:D:187:ILE:N | 2.52 | 0.41 |
| 1:D:414:GLN:OE1 | 1:D:429:PRO:HD2 | 2.21 | 0.41 |
| 1:E:193:ASN:HD22 | 1:E:389:LEU:HD22 | 1.86 | 0.41 |
| 1:E:227:ILE:HD11 | 1:E:343:ILE:HD13 | 2.02 | 0.41 |
| 1:F:12:MET:H | 1:F:12:MET:HG2 | 1.63 | 0.41 |
| 1:F:34:THR:OG1 | 1:F:35:ARG:N | 2.53 | 0.41 |
| 1:F:346:GLU:HB3 | 1:F:370:ASP:HB3 | 2.02 | 0.41 |
| 1:F:414:GLN:O | 1:F:418:GLU:HG3 | 2.21 | 0.41 |
| 1:G:119:ASP:HA | 2:G:601:XEG:HAI | 2.03 | 0.41 |
| 1:G:257:LEU:HB3 | 1:G:258:HIS:HD2 | 1.85 | 0.41 |
| 1:G:315:LEU:HD11 | 1:G:335:ASN:HB2 | 2.03 | 0.41 |
| 1:H:305:PRO:C | 1:H:307:ALA:H | 2.28 | 0.41 |
| 1:H:432:PRO:CB | 1:H:436:PHE:HD1 | 2.33 | 0.41 |
| 1:I:21:ALA:HB1 | 1:I:49:LEU:HD23 | 2.03 | 0.41 |
| 1:I:146:ARG:HG2 | 1:I:182:THR:OG1 | 2.21 | 0.41 |
| 1:J:303:GLY:O | 1:J:304:PHE:CD1 | 2.74 | 0.41 |
| 1:K:41:LYS:O | 1:K:45:VAL:HG23 | 2.21 | 0.41 |
| 1:L:350:GLY:N | 1:L:351:PRO:HD3 | 2.36 | 0.41 |
| 1:A:85:HIS:HB2 | 1:A:492:VAL:HG11 | 2.03 | 0.41 |
| 1:A:282:ASN:HD21 | 1:A:306:LYS:HB3 | 1.84 | 0.41 |
| 1:B:85:HIS:CD2 | 1:B:86:ARG:HG2 | 2.56 | 0.41 |
| 1:C:323:ILE:HG22 | 1:C:345:ALA:O | 2.21 | 0.41 |
| 1:D:315:LEU:HD22 | 1:D:322:LEU:HD21 | 2.03 | 0.41 |
| 1:E:321:ILE:HG12 | 1:E:343:ILE:HG23 | 2.02 | 0.41 |
| 1:F:8:ASN:O | 1:F:10:PHE:N | 2.52 | 0.41 |
| 1:G:14:GLU:H | 1:G:14:GLU:CD | 2.18 | 0.41 |
| 1:G:459:ARG:O | 1:G:463:GLN:HG2 | 2.21 | 0.41 |
| 1:H:18:ASP:OD1 | 1:H:53:LYS:HD3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:353:THR:OG1 | 1:H:355:GLU:HG2 | 2.21 | 0.41 |
| 1:J:233:MET:O | 1:J:237:GLY:N | 2.54 | 0.41 |
| 1:K:335:ASN:O | 1:K:338:ARG:HG2 | 2.22 | 0.41 |
| 1:L:409:LEU:HD12 | 1:L:409:LEU:HA | 1.91 | 0.41 |
| 1:A:58:VAL:HA | 1:A:80:ALA:HA | 2.03 | 0.40 |
| 1:C:369:PRO:HB3 | 1:C:478:ARG:HD3 | 2.02 | 0.40 |
| 1:D:13:VAL:HG23 | 1:D:16:PHE:HD2 | 1.86 | 0.40 |
| 1:D:378:VAL:HA | 1:D:381:SER:HB2 | 2.03 | 0.40 |
| 1:G:249:VAL:HG12 | 1:G:323:ILE:CD1 | 2.45 | 0.40 |
| 1:G:358:LYS:HA | 1:G:358:LYS:HD2 | 1.92 | 0.40 |
| 1:H:129:VAL:HG12 | 1:H:131:ILE:HG12 | 2.03 | 0.40 |
| 1:K:385:TRP:O | 1:K:389:LEU:HG | 2.21 | 0.40 |
| 1:B:226:PHE:C | 1:B:228:ASN:H | 2.28 | 0.40 |
| 1:D:379:THR:O | 1:D:382:TYR:HB3 | 2.21 | 0.40 |
| 1:E:227:ILE:HA | 1:E:233:MET:HE3 | 2.03 | 0.40 |
| 1:F:51:ILE:C | 1:F:54:PRO:HD2 | 2.46 | 0.40 |
| 1:G:201:LYS:H | 1:G:201:LYS:HG2 | 1.65 | 0.40 |
| 1:G:357:ASP:HA | 1:G:360:PHE:HB2 | 2.03 | 0.40 |
| 1:G:371:LEU:HD23 | 1:G:481:ALA:HB1 | 2.03 | 0.40 |
| 1:G:487:GLU:O | 1:G:491:ARG:HG2 | 2.20 | 0.40 |
| 1:H:88:PRO:HG2 | 1:H:122:PHE:CE2 | 2.56 | 0.40 |
| 1:H:220:PHE:CZ | 1:H:266:PHE:HE2 | 2.39 | 0.40 |
| 1:I:368:ILE:HG21 | 1:I:373:LEU:HD13 | 2.03 | 0.40 |
| 1:J:440:ILE:HA | 1:J:443:ALA:HB2 | 2.02 | 0.40 |
| 1:K:432:PRO:CB | 1:K:436:PHE:HD1 | 2.34 | 0.40 |
| 1:L:211:ARG:HD3 | 1:L:384:GLU:OE2 | 2.20 | 0.40 |
| 1:A:368:ILE:HG21 | 1:A:373:LEU:HD13 | 2.03 | 0.40 |
| 1:C:366:MET:HE2 | 1:C:475:LEU:CD2 | 2.33 | 0.40 |
| 1:D:10:PHE:HB3 | 1:D:11:LYS:H | 1.67 | 0.40 |
| 1:D:24:VAL:HG13 | 1:D:483:VAL:CG2 | 2.52 | 0.40 |
| 1:E:36:GLU:HG2 | 1:E:38:GLU:OE2 | 2.21 | 0.40 |
| 1:E:193:ASN:OD1 | 1:E:193:ASN:N | 2.54 | 0.40 |
| 1:F:114:LYS:HG2 | 1:F:371:LEU:O | 2.22 | 0.40 |
| 1:F:183:TYR:CE2 | 1:F:188:GLY:HA3 | 2.56 | 0.40 |
| 1:G:79:ARG:HA | 1:G:127:ALA:HA | 2.03 | 0.40 |
| 1:G:300:THR:CG2 | 1:G:301:ILE:N | 2.83 | 0.40 |
| 1:G:414:GLN:OE1 | 1:G:430:ILE:HG23 | 2.22 | 0.40 |
| 1:H:36:GLU:OE1 | 1:H:38:GLU:N | 2.54 | 0.40 |
| 1:H:74:VAL:HG11 | 1:K:50:ARG:O | 2.20 | 0.40 |
| 1:H:82:HIS:N | 1:H:124:GLY:O | 2.53 | 0.40 |
| 1:H:387:LYS:O | 1:H:391:HIS:N | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:319:CYS:O | 1:K:341:ALA:HA | 2.21 | 0.40 |
| 1:K:368:ILE:HG21 | 1:K:373:LEU:HD13 | 2.03 | 0.40 |
| 1:C:95:TYR:OH | 1:C:145:THR:HG22 | 2.21 | 0.40 |
| 1:F:90:LYS:HD2 | 1:F:122:PHE:CD1 | 2.56 | 0.40 |
| 1:F:315:LEU:CD2 | 1:F:322:LEU:HD21 | 2.52 | 0.40 |
| 1:I:291:LEU:HD12 | 1:I:291:LEU:HA | 1.62 | 0.40 |
| 2:I:601:XEG:CAL | 2:I:601:XEG:HAPA | 2.52 | 0.40 |
| 1:K:343:ILE:HD11 | 1:K:368:ILE:HD11 | 2.04 | 0.40 |
| 1:L:99:VAL:HA | 1:L:103:GLU:OE1 | 2.21 | 0.40 |
| 1:C:243:GLY:O | 1:C:245:LYS:N | 2.45 | 0.40 |
| 1:D:280:ILE:HD11 | 1:D:301:ILE:HD11 | 2.03 | 0.40 |
| 1:E:430:ILE:H | 1:E:430:ILE:HG13 | 1.67 | 0.40 |
| 1:F:254:ASN:H | 1:F:257:LEU:HD12 | 1.87 | 0.40 |
| 1:H:85:HIS:HB2 | 1:H:492:VAL:HG11 | 2.02 | 0.40 |
| 1:H:154:LYS:HE3 | 1:I:189:HIS:NE2 | 2.36 | 0.40 |
| 1:I:141:LEU:HD12 | 1:I:144:ILE:HD12 | 2.04 | 0.40 |
| 1:I:282:ASN:ND2 | 1:I:306:LYS:HB2 | 2.37 | 0.40 |
| 1:I:396:ARG:HB3 | 1:I:397:LEU:HD12 | 2.04 | 0.40 |
| 1:J:201:LYS:O | 1:J:211:ARG:NH2 | 2.55 | 0.40 |
| 1:K:38:GLU:O | 1:K:41:LYS:HD3 | 2.21 | 0.40 |
| 1:K:88:PRO:HG2 | 1:K:122:PHE:CD2 | 2.57 | 0.40 |
| 1:K:313:SER:OG | 1:K:314:ILE:N | 2.53 | 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 | 494/496 (100%) | 428 (87%) | 52 (10%) | 14 (3%) | 4 23 |
| 1 | B | 494/496 (100%) | 421 (85%) | 58 (12%) | 15 (3%) | 3 22 |
| 1 | C | 494/496 (100%) | 418 (85%) | 60 (12%) | 16 (3%) | 3 21 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | D | 494/496 (100%) | 423 (86%) | 55 (11%) | 16 (3%) | 3 | 21 |
| 1 | E | 494/496 (100%) | 426 (86%) | 53 (11%) | 15 (3%) | 3 | 22 |
| 1 | F | 494/496 (100%) | 420 (85%) | 59 (12%) | 15 (3%) | 3 | 22 |
| 1 | G | 494/496 (100%) | 421 (85%) | 60 (12%) | 13 (3%) | 4 | 24 |
| 1 | H | 494/496 (100%) | 420 (85%) | 61 (12%) | 13 (3%) | 4 | 24 |
| 1 | I | 494/496 (100%) | 411 (83%) | 69 (14%) | 14 (3%) | 4 | 23 |
| 1 | J | 494/496 (100%) | 420 (85%) | 58 (12%) | 16 (3%) | 3 | 21 |
| 1 | K | 494/496 (100%) | 422 (85%) | 55 (11%) | 17 (3%) | 3 | 21 |
| 1 | L | 494/496 (100%) | 418 (85%) | 66 (13%) | 10 (2%) | 6 | 29 |
| All | All | 5928/5952 (100%) | 5048 (85%) | 706 (12%) | 174 (3%) | 3 | 23 |

All (174) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 252 | PHE |
| 1 | A | 254 | ASN |
| 1 | B | 168 | ASP |
| 1 | B | 276 | SER |
| 1 | C | 12 | MET |
| 1 | D | 10 | PHE |
| 1 | D | 168 | ASP |
| 1 | E | 252 | PHE |
| 1 | F | 316 | GLU |
| 1 | G | 7 | PRO |
| 1 | G | 295 | LYS |
| 1 | H | 238 | MET |
| 1 | H | 241 | GLY |
| 1 | J | 241 | GLY |
| 1 | J | 244 | ASP |
| 1 | L | 252 | PHE |
| 1 | A | 7 | PRO |
| 1 | A | 36 | GLU |
| 1 | A | 302 | LEU |
| 1 | B | 241 | GLY |
| 1 | B | 243 | GLY |
| 1 | B | 244 | ASP |
| 1 | B | 295 | LYS |
| 1 | B | 329 | LYS |
| 1 | B | 422 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 474 | GLY |
| 1 | C | 271 | VAL |
| 1 | D | 295 | LYS |
| 1 | D | 474 | GLY |
| 1 | E | 36 | GLU |
| 1 | E | 254 | ASN |
| 1 | E | 295 | LYS |
| 1 | E | 474 | GLY |
| 1 | F | 168 | ASP |
| 1 | F | 271 | VAL |
| 1 | G | 254 | ASN |
| 1 | G | 271 | VAL |
| 1 | G | 474 | GLY |
| 1 | H | 168 | ASP |
| 1 | H | 243 | GLY |
| 1 | H | 244 | ASP |
| 1 | H | 252 | PHE |
| 1 | H | 254 | ASN |
| 1 | H | 271 | VAL |
| 1 | H | 295 | LYS |
| 1 | H | 474 | GLY |
| 1 | I | 7 | PRO |
| 1 | I | 168 | ASP |
| 1 | I | 271 | VAL |
| 1 | I | 306 | LYS |
| 1 | I | 329 | LYS |
| 1 | I | 474 | GLY |
| 1 | J | 11 | LYS |
| 1 | J | 168 | ASP |
| 1 | J | 243 | GLY |
| 1 | J | 254 | ASN |
| 1 | J | 271 | VAL |
| 1 | J | 295 | LYS |
| 1 | J | 474 | GLY |
| 1 | K | 241 | GLY |
| 1 | K | 254 | ASN |
| 1 | K | 271 | VAL |
| 1 | K | 306 | LYS |
| 1 | K | 474 | GLY |
| 1 | L | 241 | GLY |
| 1 | L | 474 | GLY |
| 1 | A | 62 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 304 | PHE |
| 1 | B | 238 | MET |
| 1 | B | 254 | ASN |
| 1 | B | 271 | VAL |
| 1 | B | 313 | SER |
| 1 | C | 254 | ASN |
| 1 | C | 291 | LEU |
| 1 | C | 295 | LYS |
| 1 | C | 327 | SER |
| 1 | D | 11 | LYS |
| 1 | D | 36 | GLU |
| 1 | D | 238 | MET |
| 1 | D | 241 | GLY |
| 1 | D | 254 | ASN |
| 1 | D | 313 | SER |
| 1 | E | 168 | ASP |
| 1 | F | 82 | HIS |
| 1 | F | 254 | ASN |
| 1 | F | 295 | LYS |
| 1 | G | 168 | ASP |
| 1 | G | 244 | ASP |
| 1 | G | 252 | PHE |
| 1 | H | 11 | LYS |
| 1 | I | 252 | PHE |
| 1 | J | 82 | HIS |
| 1 | J | 318 | ASP |
| 1 | K | 82 | HIS |
| 1 | L | 168 | ASP |
| 1 | L | 187 | ILE |
| 1 | A | 168 | ASP |
| 1 | A | 295 | LYS |
| 1 | A | 474 | GLY |
| 1 | C | 7 | PRO |
| 1 | C | 11 | LYS |
| 1 | C | 58 | VAL |
| 1 | D | 243 | GLY |
| 1 | D | 276 | SER |
| 1 | E | 37 | THR |
| 1 | E | 38 | GLU |
| 1 | E | 302 | LEU |
| 1 | F | 9 | PHE |
| 1 | F | 88 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 82 | HIS |
| 1 | I | 36 | GLU |
| 1 | J | 238 | MET |
| 1 | J | 338 | ARG |
| 1 | K | 10 | PHE |
| 1 | K | 227 | ILE |
| 1 | K | 243 | GLY |
| 1 | K | 295 | LYS |
| 1 | K | 335 | ASN |
| 1 | L | 36 | GLU |
| 1 | L | 295 | LYS |
| 1 | A | 8 | ASN |
| 1 | A | 243 | GLY |
| 1 | A | 271 | VAL |
| 1 | A | 339 | VAL |
| 1 | B | 11 | LYS |
| 1 | C | 82 | HIS |
| 1 | C | 168 | ASP |
| 1 | C | 244 | ASP |
| 1 | C | 329 | LYS |
| 1 | C | 339 | VAL |
| 1 | D | 271 | VAL |
| 1 | E | 227 | ILE |
| 1 | E | 329 | LYS |
| 1 | E | 339 | VAL |
| 1 | F | 339 | VAL |
| 1 | F | 474 | GLY |
| 1 | G | 82 | HIS |
| 1 | H | 339 | VAL |
| 1 | I | 82 | HIS |
| 1 | I | 227 | ILE |
| 1 | I | 254 | ASN |
| 1 | I | 339 | VAL |
| 1 | J | 339 | VAL |
| 1 | K | 36 | GLU |
| 1 | K | 257 | LEU |
| 1 | L | 271 | VAL |
| 1 | L | 339 | VAL |
| 1 | C | 243 | GLY |
| 1 | C | 425 | GLY |
| 1 | D | 7 | PRO |
| 1 | E | 62 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 241 | GLY |
| 1 | I | 295 | LYS |
| 1 | J | 58 | VAL |
| 1 | K | 244 | ASP |
| 1 | L | 254 | ASN |
| 1 | B | 339 | VAL |
| 1 | E | 271 | VAL |
| 1 | D | 339 | VAL |
| 1 | F | 227 | ILE |
| 1 | F | 241 | GLY |
| 1 | F | 243 | GLY |
| 1 | G | 339 | VAL |
| 1 | J | 165 | PRO |
| 1 | K | 299 | GLY |
| 1 | K | 339 | VAL |
| 1 | E | 187 | ILE |
| 1 | F | 187 | ILE |
| 1 | F | 299 | GLY |
| 1 | I | 187 | ILE |
| 1 | K | 158 | ILE |
| 1 | D | 165 | PRO |
| 1 | G | 88 | PRO |
| 1 | G | 299 | GLY |

### 5.3.2 Protein sidechains (i)

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 | 413/413 (100%) | 413 (100%) | 0 | 100 100 |
| 1 | B | 413/413 (100%) | 412 (100%) | 1 (0%) | 87 84 |
| 1 | C | 413/413 (100%) | 413 (100%) | 0 | 100 100 |
| 1 | D | 413/413 (100%) | 413 (100%) | 0 | 100 100 |
| 1 | E | 413/413 (100%) | 413 (100%) | 0 | 100 100 |
| 1 | F | 413/413 (100%) | 412 (100%) | 1 (0%) | 87 84 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | G | 413/413 (100%) | 413 (100%) | 0 | 100 | 100 |
| 1 | H | 413/413 (100%) | 413 (100%) | 0 | 100 | 100 |
| 1 | I | 413/413 (100%) | 413 (100%) | 0 | 100 | 100 |
| 1 | J | 413/413 (100%) | 413 (100%) | 0 | 100 | 100 |
| 1 | K | 413/413 (100%) | 413 (100%) | 0 | 100 | 100 |
| 1 | L | 413/413 (100%) | 413 (100%) | 0 | 100 | 100 |
| All | All | 4956/4956 (100%) | 4954 (100%) | 2 (0%) | 100 | 100 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 158 | ILE |
| 1 | F | 493 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 298 | HIS |
| 1 | A | 364 | ASN |
| 1 | A | 390 | ASN |
| 1 | A | 391 | HIS |
| 1 | A | 494 | ASN |
| 1 | B | 56 | ASN |
| 1 | B | 189 | HIS |
| 1 | B | 298 | HIS |
| 1 | C | 56 | ASN |
| 1 | C | 84 | GLN |
| 1 | C | 209 | HIS |
| 1 | C | 264 | HIS |
| 1 | D | 193 | ASN |
| 1 | D | 330 | GLN |
| 1 | D | 463 | GLN |
| 1 | E | 189 | HIS |
| 1 | E | 250 | GLN |
| 1 | E | 494 | ASN |
| 1 | F | 84 | GLN |
| 1 | F | 209 | HIS |
| 1 | F | 298 | HIS |
| 1 | G | 195 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 330 | GLN |
| 1 | G | 349 | ASN |
| 1 | H | 189 | HIS |
| 1 | H | 195 | HIS |
| 1 | I | 43 | ASN |
| 1 | I | 56 | ASN |
| 1 | I | 84 | GLN |
| 1 | I | 193 | ASN |
| 1 | I | 195 | HIS |
| 1 | I | 364 | ASN |
| 1 | I | 391 | HIS |
| 1 | I | 450 | HIS |
| 1 | J | 205 | GLN |
| 1 | J | 390 | ASN |
| 1 | K | 258 | HIS |
| 1 | K | 298 | HIS |
| 1 | K | 330 | GLN |
| 1 | K | 364 | ASN |
| 1 | K | 494 | ASN |
| 1 | L | 82 | HIS |
| 1 | L | 84 | GLN |
| 1 | L | 193 | ASN |
| 1 | L | 225 | ASN |
| 1 | L | 330 | GLN |
| 1 | L | 388 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

12 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 | $\#\|Z\| > 2$ |
| 2 | XEG | C | 601 | - | 35,35,35 | 2.34 | 12 (34%) | 52,52,52 | 1.97 | 16 (30%) |
| 2 | XEG | E | 601 | - | 35,35,35 | 2.25 | 13 (37%) | 52,52,52 | 1.87 | 13 (25%) |
| 2 | XEG | G | 601 | - | 35,35,35 | 2.30 | 12 (34%) | 52,52,52 | 1.90 | 14 (26%) |
| 2 | XEG | I | 601 | - | 35,35,35 | 2.34 | 12 (34%) | 52,52,52 | 1.96 | 13 (25%) |
| 2 | XEG | F | 601 | - | 35,35,35 | 2.34 | 12 (34%) | 52,52,52 | 1.96 | 16 (30%) |
| 2 | XEG | B | 601 | - | 35,35,35 | 2.28 | 11 (31%) | 52,52,52 | 1.97 | 15 (28%) |
| 2 | XEG | J | 601 | - | 35,35,35 | 2.28 | 11 (31%) | 52,52,52 | 1.94 | 13 (25%) |
| 2 | XEG | A | 601 | - | 35,35,35 | 2.27 | 13 (37%) | 52,52,52 | 1.88 | 15 (28%) |
| 2 | XEG | D | 601 | - | 35,35,35 | 2.26 | 11 (31%) | 52,52,52 | 1.93 | 13 (25%) |
| 2 | XEG | L | 601 | - | 35,35,35 | 2.34 | 10 (28%) | 52,52,52 | 1.92 | 14 (26%) |
| 2 | XEG | H | 601 | - | 35,35,35 | 2.31 | 11 (31%) | 52,52,52 | 1.96 | 16 (30%) |
| 2 | XEG | K | 601 | - | 35,35,35 | 2.28 | 13 (37%) | 52,52,52 | 1.86 | 14 (26%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | XEG | C | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | E | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | G | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | I | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | F | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | B | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | J | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | A | 601 | - | - | 8/12/24/24 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | XEG | D | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | L | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | H | 601 | - | - | 8/12/24/24 | 0/4/4/4 |
| 2 | XEG | K | 601 | - | - | 8/12/24/24 | 0/4/4/4 |

All (141) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 601 | XEG | OAR-CBC | 9.12 | 1.50 | 1.38 |
| 2 | C | 601 | XEG | OAR-CBC | 9.05 | 1.50 | 1.38 |
| 2 | L | 601 | XEG | OAR-CBC | 9.02 | 1.50 | 1.38 |
| 2 | F | 601 | XEG | OAR-CBC | 8.91 | 1.50 | 1.38 |
| 2 | B | 601 | XEG | OAR-CBC | 8.80 | 1.50 | 1.38 |
| 2 | H | 601 | XEG | OAR-CBC | 8.78 | 1.50 | 1.38 |
| 2 | J | 601 | XEG | OAR-CBC | 8.78 | 1.49 | 1.38 |
| 2 | G | 601 | XEG | OAR-CBC | 8.71 | 1.49 | 1.38 |
| 2 | D | 601 | XEG | OAR-CBC | 8.71 | 1.49 | 1.38 |
| 2 | A | 601 | XEG | OAR-CBC | 8.70 | 1.49 | 1.38 |
| 2 | K | 601 | XEG | OAR-CBC | 8.69 | 1.49 | 1.38 |
| 2 | E | 601 | XEG | OAR-CBC | 8.54 | 1.49 | 1.38 |
| 2 | L | 601 | XEG | OAC-CAU | 4.26 | 1.44 | 1.36 |
| 2 | F | 601 | XEG | OAC-CAU | 4.24 | 1.44 | 1.36 |
| 2 | J | 601 | XEG | OAC-CAU | 4.20 | 1.44 | 1.36 |
| 2 | I | 601 | XEG | OAC-CAU | 4.17 | 1.44 | 1.36 |
| 2 | B | 601 | XEG | OAC-CAU | 4.16 | 1.44 | 1.36 |
| 2 | C | 601 | XEG | OAC-CAU | 4.16 | 1.44 | 1.36 |
| 2 | H | 601 | XEG | OAC-CAU | 4.15 | 1.44 | 1.36 |
| 2 | D | 601 | XEG | OAC-CAU | 4.07 | 1.44 | 1.36 |
| 2 | G | 601 | XEG | OAC-CAU | 4.02 | 1.44 | 1.36 |
| 2 | E | 601 | XEG | OAC-CAU | 3.99 | 1.44 | 1.36 |
| 2 | A | 601 | XEG | OAC-CAU | 3.99 | 1.44 | 1.36 |
| 2 | K | 601 | XEG | OAC-CAU | 3.89 | 1.44 | 1.36 |
| 2 | B | 601 | XEG | OAB-CAT | 3.71 | 1.45 | 1.37 |
| 2 | I | 601 | XEG | OAB-CAT | 3.70 | 1.45 | 1.37 |
| 2 | D | 601 | XEG | OAB-CAT | 3.69 | 1.45 | 1.37 |
| 2 | C | 601 | XEG | OAB-CAT | 3.68 | 1.45 | 1.37 |
| 2 | F | 601 | XEG | OAB-CAT | 3.67 | 1.45 | 1.37 |
| 2 | A | 601 | XEG | OAB-CAT | 3.67 | 1.45 | 1.37 |
| 2 | E | 601 | XEG | OAB-CAT | 3.65 | 1.45 | 1.37 |
| 2 | L | 601 | XEG | OAB-CAT | 3.65 | 1.45 | 1.37 |
| 2 | G | 601 | XEG | OAB-CAT | 3.64 | 1.45 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 601 | XEG | OAB-CAT | 3.61 | 1.45 | 1.37 |
| 2 | H | 601 | XEG | OAB-CAT | 3.61 | 1.45 | 1.37 |
| 2 | K | 601 | XEG | OAB-CAT | 3.59 | 1.45 | 1.37 |
| 2 | G | 601 | XEG | OAH-CBB | 3.23 | 1.44 | 1.36 |
| 2 | K | 601 | XEG | OAH-CBB | 3.21 | 1.44 | 1.36 |
| 2 | I | 601 | XEG | OAH-CBB | 3.20 | 1.44 | 1.36 |
| 2 | L | 601 | XEG | OAH-CBB | 3.20 | 1.44 | 1.36 |
| 2 | F | 601 | XEG | CAP-CBE | -3.18 | 1.45 | 1.51 |
| 2 | A | 601 | XEG | OAH-CBB | 3.16 | 1.44 | 1.36 |
| 2 | F | 601 | XEG | OAH-CBB | 3.15 | 1.44 | 1.36 |
| 2 | C | 601 | XEG | CAP-CBE | -3.14 | 1.45 | 1.51 |
| 2 | E | 601 | XEG | OAH-CBB | 3.14 | 1.44 | 1.36 |
| 2 | H | 601 | XEG | OAH-CBB | 3.13 | 1.44 | 1.36 |
| 2 | H | 601 | XEG | CAP-CBE | -3.12 | 1.45 | 1.51 |
| 2 | D | 601 | XEG | OAH-CBB | 3.11 | 1.44 | 1.36 |
| 2 | K | 601 | XEG | CAP-CBE | -3.08 | 1.45 | 1.51 |
| 2 | G | 601 | XEG | CAP-CBE | -3.06 | 1.45 | 1.51 |
| 2 | B | 601 | XEG | OAH-CBB | 3.06 | 1.43 | 1.36 |
| 2 | F | 601 | XEG | CAZ-CAS | 3.04 | 1.56 | 1.50 |
| 2 | J | 601 | XEG | OAH-CBB | 3.03 | 1.43 | 1.36 |
| 2 | C | 601 | XEG | OAH-CBB | 3.02 | 1.43 | 1.36 |
| 2 | L | 601 | XEG | CAP-CBE | -2.97 | 1.46 | 1.51 |
| 2 | L | 601 | XEG | OAD-CAV | 2.97 | 1.42 | 1.36 |
| 2 | H | 601 | XEG | OAD-CAV | 2.96 | 1.42 | 1.36 |
| 2 | F | 601 | XEG | OAD-CAV | 2.95 | 1.42 | 1.36 |
| 2 | C | 601 | XEG | OAD-CAV | 2.94 | 1.42 | 1.36 |
| 2 | I | 601 | XEG | OAD-CAV | 2.93 | 1.42 | 1.36 |
| 2 | J | 601 | XEG | CAP-CBE | -2.91 | 1.46 | 1.51 |
| 2 | A | 601 | XEG | CAP-CBE | -2.90 | 1.46 | 1.51 |
| 2 | B | 601 | XEG | CAP-CBE | -2.90 | 1.46 | 1.51 |
| 2 | D | 601 | XEG | OAD-CAV | 2.88 | 1.42 | 1.36 |
| 2 | G | 601 | XEG | OAD-CAV | 2.87 | 1.42 | 1.36 |
| 2 | C | 601 | XEG | CAZ-CAS | 2.86 | 1.56 | 1.50 |
| 2 | E | 601 | XEG | CAP-CBE | -2.85 | 1.46 | 1.51 |
| 2 | B | 601 | XEG | OAD-CAV | 2.85 | 1.42 | 1.36 |
| 2 | E | 601 | XEG | OAD-CAV | 2.84 | 1.42 | 1.36 |
| 2 | A | 601 | XEG | OAD-CAV | 2.84 | 1.42 | 1.36 |
| 2 | K | 601 | XEG | OAD-CAV | 2.83 | 1.42 | 1.36 |
| 2 | J | 601 | XEG | OAD-CAV | 2.82 | 1.42 | 1.36 |
| 2 | D | 601 | XEG | CAP-CBE | -2.81 | 1.46 | 1.51 |
| 2 | G | 601 | XEG | CAZ-CAS | 2.80 | 1.56 | 1.50 |
| 2 | K | 601 | XEG | CAZ-CAS | 2.79 | 1.56 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | H | 601 | XEG | CAZ-CAS | 2.77 | 1.56 | 1.50 |
| 2 | I | 601 | XEG | CAP-CBE | -2.77 | 1.46 | 1.51 |
| 2 | L | 601 | XEG | OAG-CAY | 2.76 | 1.41 | 1.36 |
| 2 | L | 601 | XEG | CAZ-CAS | 2.75 | 1.56 | 1.50 |
| 2 | E | 601 | XEG | OAG-CAY | 2.75 | 1.41 | 1.36 |
| 2 | J | 601 | XEG | OAG-CAY | 2.74 | 1.41 | 1.36 |
| 2 | G | 601 | XEG | OAG-CAY | 2.74 | 1.41 | 1.36 |
| 2 | I | 601 | XEG | OAG-CAY | 2.74 | 1.41 | 1.36 |
| 2 | C | 601 | XEG | OAG-CAY | 2.73 | 1.41 | 1.36 |
| 2 | A | 601 | XEG | OAG-CAY | 2.73 | 1.41 | 1.36 |
| 2 | F | 601 | XEG | OAG-CAY | 2.73 | 1.41 | 1.36 |
| 2 | K | 601 | XEG | OAG-CAY | 2.71 | 1.41 | 1.36 |
| 2 | H | 601 | XEG | OAG-CAY | 2.70 | 1.41 | 1.36 |
| 2 | I | 601 | XEG | CAZ-CAS | 2.68 | 1.56 | 1.50 |
| 2 | B | 601 | XEG | OAG-CAY | 2.67 | 1.41 | 1.36 |
| 2 | D | 601 | XEG | OAG-CAY | 2.66 | 1.41 | 1.36 |
| 2 | E | 601 | XEG | CAZ-CAS | 2.64 | 1.55 | 1.50 |
| 2 | J | 601 | XEG | CAZ-CAS | 2.63 | 1.55 | 1.50 |
| 2 | A | 601 | XEG | CAZ-CAS | 2.60 | 1.55 | 1.50 |
| 2 | B | 601 | XEG | CAZ-CAS | 2.58 | 1.55 | 1.50 |
| 2 | D | 601 | XEG | CAZ-CAS | 2.57 | 1.55 | 1.50 |
| 2 | L | 601 | XEG | CAK-CAT | 2.45 | 1.42 | 1.39 |
| 2 | I | 601 | XEG | OAQ-CAS | 2.41 | 1.39 | 1.34 |
| 2 | C | 601 | XEG | CAK-CAT | 2.37 | 1.42 | 1.39 |
| 2 | K | 601 | XEG | CAK-CAT | 2.36 | 1.42 | 1.39 |
| 2 | H | 601 | XEG | OAQ-CAS | 2.35 | 1.39 | 1.34 |
| 2 | I | 601 | XEG | CAK-CAT | 2.34 | 1.42 | 1.39 |
| 2 | F | 601 | XEG | CAK-CAT | 2.33 | 1.42 | 1.39 |
| 2 | E | 601 | XEG | CAK-CAT | 2.32 | 1.42 | 1.39 |
| 2 | G | 601 | XEG | CAK-CAT | 2.30 | 1.42 | 1.39 |
| 2 | A | 601 | XEG | CAK-CAT | 2.30 | 1.42 | 1.39 |
| 2 | J | 601 | XEG | CAK-CAT | 2.27 | 1.42 | 1.39 |
| 2 | L | 601 | XEG | OAE-CAW | 2.27 | 1.40 | 1.36 |
| 2 | C | 601 | XEG | OAE-CAW | 2.27 | 1.40 | 1.36 |
| 2 | D | 601 | XEG | CAK-CAT | 2.26 | 1.42 | 1.39 |
| 2 | B | 601 | XEG | OAE-CAW | 2.26 | 1.40 | 1.36 |
| 2 | J | 601 | XEG | OAQ-CAS | 2.25 | 1.39 | 1.34 |
| 2 | G | 601 | XEG | OAQ-CAS | 2.25 | 1.39 | 1.34 |
| 2 | F | 601 | XEG | OAE-CAW | 2.25 | 1.40 | 1.36 |
| 2 | H | 601 | XEG | OAE-CAW | 2.25 | 1.40 | 1.36 |
| 2 | E | 601 | XEG | OAE-CAW | 2.24 | 1.40 | 1.36 |
| 2 | B | 601 | XEG | OAQ-CAS | 2.24 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | H | 601 | XEG | CAK-CAT | 2.24 | 1.42 | 1.39 |
| 2 | I | 601 | XEG | OAE-CAW | 2.24 | 1.40 | 1.36 |
| 2 | A | 601 | XEG | OAE-CAW | 2.23 | 1.40 | 1.36 |
| 2 | G | 601 | XEG | OAE-CAW | 2.23 | 1.40 | 1.36 |
| 2 | D | 601 | XEG | OAE-CAW | 2.21 | 1.40 | 1.36 |
| 2 | J | 601 | XEG | OAE-CAW | 2.20 | 1.40 | 1.36 |
| 2 | K | 601 | XEG | OAE-CAW | 2.20 | 1.40 | 1.36 |
| 2 | E | 601 | XEG | OAQ-CAS | 2.16 | 1.39 | 1.34 |
| 2 | K | 601 | XEG | OAQ-CAS | 2.15 | 1.39 | 1.34 |
| 2 | F | 601 | XEG | OAQ-CAS | 2.15 | 1.39 | 1.34 |
| 2 | A | 601 | XEG | CBC-CBD | 2.14 | 1.43 | 1.40 |
| 2 | B | 601 | XEG | CAK-CAT | 2.13 | 1.42 | 1.39 |
| 2 | G | 601 | XEG | CBC-CBD | 2.12 | 1.43 | 1.40 |
| 2 | A | 601 | XEG | OAR-CBF | -2.10 | 1.42 | 1.45 |
| 2 | D | 601 | XEG | OAQ-CAS | 2.10 | 1.39 | 1.34 |
| 2 | E | 601 | XEG | CBC-CBD | 2.08 | 1.43 | 1.40 |
| 2 | C | 601 | XEG | OAQ-CAS | 2.06 | 1.38 | 1.34 |
| 2 | E | 601 | XEG | OAR-CBF | -2.05 | 1.42 | 1.45 |
| 2 | A | 601 | XEG | OAQ-CAS | 2.05 | 1.38 | 1.34 |
| 2 | K | 601 | XEG | CBC-CBD | 2.04 | 1.43 | 1.40 |
| 2 | I | 601 | XEG | CBC-CBD | 2.03 | 1.43 | 1.40 |
| 2 | K | 601 | XEG | OAR-CBF | -2.03 | 1.42 | 1.45 |
| 2 | F | 601 | XEG | CBC-CBD | 2.00 | 1.43 | 1.40 |
| 2 | C | 601 | XEG | CBC-CBD | 2.00 | 1.43 | 1.40 |

All (172) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 601 | XEG | OAQ-CAS-CAZ | 6.40 | 122.18 | 111.90 |
| 2 | C | 601 | XEG | OAQ-CAS-CAZ | 5.69 | 121.04 | 111.90 |
| 2 | G | 601 | XEG | OAQ-CAS-CAZ | 5.37 | 120.53 | 111.90 |
| 2 | J | 601 | XEG | OAG-CAY-CBD | 5.24 | 129.99 | 117.81 |
| 2 | D | 601 | XEG | OAG-CAY-CBD | 5.24 | 129.99 | 117.81 |
| 2 | E | 601 | XEG | OAG-CAY-CBD | 5.22 | 129.94 | 117.81 |
| 2 | K | 601 | XEG | OAG-CAY-CBD | 5.18 | 129.85 | 117.81 |
| 2 | B | 601 | XEG | OAG-CAY-CBD | 5.15 | 129.78 | 117.81 |
| 2 | H | 601 | XEG | OAG-CAY-CBD | 5.13 | 129.75 | 117.81 |
| 2 | G | 601 | XEG | OAG-CAY-CBD | 5.11 | 129.70 | 117.81 |
| 2 | L | 601 | XEG | OAG-CAY-CBD | 5.10 | 129.67 | 117.81 |
| 2 | I | 601 | XEG | OAG-CAY-CBD | 5.10 | 129.67 | 117.81 |
| 2 | A | 601 | XEG | OAG-CAY-CBD | 5.09 | 129.64 | 117.81 |
| 2 | C | 601 | XEG | OAG-CAY-CBD | 5.03 | 129.51 | 117.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 601 | XEG | OAG-CAY-CBD | 5.01 | 129.47 | 117.81 |
| 2 | H | 601 | XEG | OAQ-CAS-CAZ | 4.97 | 119.88 | 111.90 |
| 2 | L | 601 | XEG | OAQ-CAS-CAZ | 4.69 | 119.43 | 111.90 |
| 2 | K | 601 | XEG | OAQ-CAS-CAZ | 4.67 | 119.41 | 111.90 |
| 2 | I | 601 | XEG | CBD-CAP-CBE | 4.55 | 122.74 | 111.48 |
| 2 | E | 601 | XEG | OAQ-CAS-CAZ | 4.49 | 119.11 | 111.90 |
| 2 | I | 601 | XEG | OAQ-CAS-CAZ | 4.30 | 118.80 | 111.90 |
| 2 | B | 601 | XEG | OAQ-CAS-CAZ | 4.20 | 118.65 | 111.90 |
| 2 | C | 601 | XEG | OAR-CBC-CAN | 4.17 | 123.41 | 116.29 |
| 2 | F | 601 | XEG | OAR-CBC-CAN | 4.17 | 123.41 | 116.29 |
| 2 | J | 601 | XEG | OAR-CBC-CAN | 4.13 | 123.34 | 116.29 |
| 2 | H | 601 | XEG | OAR-CBC-CAN | 4.11 | 123.31 | 116.29 |
| 2 | E | 601 | XEG | OAG-CAY-CAK | -4.06 | 108.49 | 119.45 |
| 2 | B | 601 | XEG | OAR-CBC-CAN | 4.05 | 123.22 | 116.29 |
| 2 | A | 601 | XEG | OAG-CAY-CAK | -4.05 | 108.52 | 119.45 |
| 2 | A | 601 | XEG | OAQ-CAS-CAZ | 4.04 | 118.40 | 111.90 |
| 2 | I | 601 | XEG | OAG-CAY-CAK | -4.03 | 108.58 | 119.45 |
| 2 | L | 601 | XEG | OAR-CBC-CAN | 4.01 | 123.14 | 116.29 |
| 2 | D | 601 | XEG | OAR-CBC-CAN | 4.00 | 123.12 | 116.29 |
| 2 | D | 601 | XEG | OAG-CAY-CAK | -3.98 | 108.70 | 119.45 |
| 2 | G | 601 | XEG | OAG-CAY-CAK | -3.96 | 108.76 | 119.45 |
| 2 | J | 601 | XEG | OAG-CAY-CAK | -3.95 | 108.80 | 119.45 |
| 2 | B | 601 | XEG | OAG-CAY-CAK | -3.93 | 108.84 | 119.45 |
| 2 | K | 601 | XEG | OAG-CAY-CAK | -3.91 | 108.91 | 119.45 |
| 2 | I | 601 | XEG | OAR-CBC-CAN | 3.90 | 122.96 | 116.29 |
| 2 | L | 601 | XEG | OAG-CAY-CAK | -3.90 | 108.93 | 119.45 |
| 2 | K | 601 | XEG | OAR-CBC-CAN | 3.88 | 122.92 | 116.29 |
| 2 | B | 601 | XEG | CBD-CAP-CBE | 3.87 | 121.06 | 111.48 |
| 2 | H | 601 | XEG | OAG-CAY-CAK | -3.87 | 109.01 | 119.45 |
| 2 | C | 601 | XEG | OAG-CAY-CAK | -3.84 | 109.09 | 119.45 |
| 2 | F | 601 | XEG | OAG-CAY-CAK | -3.80 | 109.19 | 119.45 |
| 2 | G | 601 | XEG | OAR-CBC-CAN | 3.75 | 122.69 | 116.29 |
| 2 | E | 601 | XEG | OAR-CBC-CAN | 3.74 | 122.67 | 116.29 |
| 2 | A | 601 | XEG | OAR-CBC-CAN | 3.73 | 122.66 | 116.29 |
| 2 | D | 601 | XEG | CAL-CAZ-CAS | -3.70 | 112.89 | 120.09 |
| 2 | D | 601 | XEG | CBD-CAP-CBE | 3.69 | 120.61 | 111.48 |
| 2 | D | 601 | XEG | OAQ-CAS-CAZ | 3.68 | 117.81 | 111.90 |
| 2 | B | 601 | XEG | CAL-CAZ-CAS | -3.64 | 113.02 | 120.09 |
| 2 | B | 601 | XEG | OAB-CAT-CAK | -3.58 | 110.50 | 119.85 |
| 2 | H | 601 | XEG | OAB-CAT-CAK | -3.57 | 110.52 | 119.85 |
| 2 | C | 601 | XEG | OAB-CAT-CAK | -3.56 | 110.53 | 119.85 |
| 2 | A | 601 | XEG | CBD-CAP-CBE | 3.55 | 120.26 | 111.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 601 | XEG | OAB-CAT-CAK | -3.54 | 110.59 | 119.85 |
| 2 | J | 601 | XEG | OAB-CAT-CAK | -3.53 | 110.62 | 119.85 |
| 2 | G | 601 | XEG | OAB-CAT-CAK | -3.51 | 110.66 | 119.85 |
| 2 | D | 601 | XEG | OAB-CAT-CAK | -3.51 | 110.67 | 119.85 |
| 2 | K | 601 | XEG | OAB-CAT-CAK | -3.51 | 110.67 | 119.85 |
| 2 | J | 601 | XEG | OAQ-CAS-CAZ | 3.49 | 117.51 | 111.90 |
| 2 | I | 601 | XEG | OAB-CAT-CAK | -3.47 | 110.76 | 119.85 |
| 2 | J | 601 | XEG | CBD-CAP-CBE | 3.44 | 120.01 | 111.48 |
| 2 | J | 601 | XEG | CAL-CAZ-CAS | -3.44 | 113.40 | 120.09 |
| 2 | H | 601 | XEG | CBD-CAP-CBE | 3.43 | 119.97 | 111.48 |
| 2 | L | 601 | XEG | CBD-CAP-CBE | 3.43 | 119.96 | 111.48 |
| 2 | E | 601 | XEG | OAB-CAT-CAK | -3.41 | 110.93 | 119.85 |
| 2 | L | 601 | XEG | OAB-CAT-CAK | -3.37 | 111.03 | 119.85 |
| 2 | B | 601 | XEG | OAB-CAT-CAN | 3.36 | 128.65 | 119.85 |
| 2 | A | 601 | XEG | OAB-CAT-CAK | -3.36 | 111.07 | 119.85 |
| 2 | G | 601 | XEG | CBD-CAP-CBE | 3.35 | 119.78 | 111.48 |
| 2 | C | 601 | XEG | CBD-CAP-CBE | 3.33 | 119.73 | 111.48 |
| 2 | E | 601 | XEG | CBD-CAP-CBE | 3.31 | 119.67 | 111.48 |
| 2 | D | 601 | XEG | OAB-CAT-CAN | 3.30 | 128.50 | 119.85 |
| 2 | J | 601 | XEG | OAB-CAT-CAN | 3.30 | 128.49 | 119.85 |
| 2 | H | 601 | XEG | OAB-CAT-CAN | 3.28 | 128.44 | 119.85 |
| 2 | F | 601 | XEG | OAB-CAT-CAN | 3.28 | 128.44 | 119.85 |
| 2 | I | 601 | XEG | OAB-CAT-CAN | 3.28 | 128.43 | 119.85 |
| 2 | C | 601 | XEG | OAB-CAT-CAN | 3.27 | 128.42 | 119.85 |
| 2 | I | 601 | XEG | CAL-CAZ-CAS | -3.26 | 113.76 | 120.09 |
| 2 | A | 601 | XEG | OAB-CAT-CAN | 3.25 | 128.37 | 119.85 |
| 2 | E | 601 | XEG | OAB-CAT-CAN | 3.24 | 128.33 | 119.85 |
| 2 | K | 601 | XEG | OAB-CAT-CAN | 3.22 | 128.29 | 119.85 |
| 2 | J | 601 | XEG | OAR-CBC-CBD | -3.22 | 116.76 | 122.20 |
| 2 | G | 601 | XEG | OAB-CAT-CAN | 3.22 | 128.29 | 119.85 |
| 2 | H | 601 | XEG | CAL-CAZ-CAS | -3.21 | 113.84 | 120.09 |
| 2 | F | 601 | XEG | OAR-CBC-CBD | -3.20 | 116.80 | 122.20 |
| 2 | L | 601 | XEG | OAB-CAT-CAN | 3.15 | 128.11 | 119.85 |
| 2 | K | 601 | XEG | OAR-CBC-CBD | -3.15 | 116.89 | 122.20 |
| 2 | D | 601 | XEG | CAM-CAZ-CAS | 3.13 | 126.17 | 120.09 |
| 2 | H | 601 | XEG | OAR-CBC-CBD | -3.11 | 116.96 | 122.20 |
| 2 | C | 601 | XEG | OAR-CBC-CBD | -3.09 | 116.98 | 122.20 |
| 2 | D | 601 | XEG | OAR-CBC-CBD | -3.08 | 117.00 | 122.20 |
| 2 | B | 601 | XEG | CAM-CAZ-CAS | 3.07 | 126.06 | 120.09 |
| 2 | E | 601 | XEG | OAR-CBC-CBD | -3.05 | 117.05 | 122.20 |
| 2 | A | 601 | XEG | OAR-CBC-CBD | -3.01 | 117.13 | 122.20 |
| 2 | B | 601 | XEG | OAR-CBC-CBD | -3.00 | 117.14 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | L | 601 | XEG | OAR-CBC-CBD | -2.93 | 117.25 | 122.20 |
| 2 | A | 601 | XEG | CAL-CAZ-CAS | -2.90 | 114.45 | 120.09 |
| 2 | K | 601 | XEG | CBD-CAP-CBE | 2.87 | 118.59 | 111.48 |
| 2 | J | 601 | XEG | CAP-CBD-CBC | -2.86 | 116.32 | 121.01 |
| 2 | G | 601 | XEG | OAR-CBC-CBD | -2.85 | 117.38 | 122.20 |
| 2 | L | 601 | XEG | CAL-CAZ-CAS | -2.84 | 114.57 | 120.09 |
| 2 | E | 601 | XEG | CAL-CAZ-CAS | -2.82 | 114.61 | 120.09 |
| 2 | L | 601 | XEG | CAP-CBE-CBF | 2.82 | 115.91 | 110.16 |
| 2 | I | 601 | XEG | CAM-CAZ-CAS | 2.80 | 125.54 | 120.09 |
| 2 | F | 601 | XEG | OAQ-CAS-OAA | -2.80 | 119.00 | 123.55 |
| 2 | G | 601 | XEG | CAP-CBE-CBF | 2.79 | 115.85 | 110.16 |
| 2 | L | 601 | XEG | CAP-CBD-CBC | -2.76 | 116.48 | 121.01 |
| 2 | H | 601 | XEG | CAM-CAZ-CAS | 2.75 | 125.44 | 120.09 |
| 2 | J | 601 | XEG | CAM-CAZ-CAS | 2.71 | 125.36 | 120.09 |
| 2 | I | 601 | XEG | OAR-CBC-CBD | -2.70 | 117.63 | 122.20 |
| 2 | F | 601 | XEG | CAP-CBD-CBC | -2.69 | 116.60 | 121.01 |
| 2 | A | 601 | XEG | CAP-CBE-CBF | 2.68 | 115.62 | 110.16 |
| 2 | F | 601 | XEG | CBD-CAP-CBE | 2.64 | 118.03 | 111.48 |
| 2 | C | 601 | XEG | CAP-CBE-CBF | 2.61 | 115.49 | 110.16 |
| 2 | C | 601 | XEG | CAP-CBD-CBC | -2.60 | 116.75 | 121.01 |
| 2 | I | 601 | XEG | CAP-CBE-CBF | 2.59 | 115.46 | 110.16 |
| 2 | E | 601 | XEG | CAP-CBE-CBF | 2.55 | 115.37 | 110.16 |
| 2 | B | 601 | XEG | OAR-CBF-CBE | 2.54 | 115.99 | 109.13 |
| 2 | G | 601 | XEG | OAR-CBF-CBE | 2.53 | 115.96 | 109.13 |
| 2 | A | 601 | XEG | OAR-CBF-CBE | 2.52 | 115.91 | 109.13 |
| 2 | K | 601 | XEG | CAP-CBD-CBC | -2.51 | 116.90 | 121.01 |
| 2 | I | 601 | XEG | OAR-CBF-CBE | 2.51 | 115.88 | 109.13 |
| 2 | H | 601 | XEG | CAP-CBD-CBC | -2.50 | 116.90 | 121.01 |
| 2 | D | 601 | XEG | CAP-CBD-CBC | -2.50 | 116.91 | 121.01 |
| 2 | L | 601 | XEG | CAM-CAZ-CAS | 2.50 | 124.95 | 120.09 |
| 2 | D | 601 | XEG | CAP-CBE-CBF | 2.49 | 115.25 | 110.16 |
| 2 | K | 601 | XEG | OAR-CBF-CBE | 2.47 | 115.78 | 109.13 |
| 2 | K | 601 | XEG | CAP-CBE-CBF | 2.45 | 115.16 | 110.16 |
| 2 | H | 601 | XEG | CAP-CBE-CBF | 2.43 | 115.12 | 110.16 |
| 2 | G | 601 | XEG | CAL-CAZ-CAS | -2.43 | 115.37 | 120.09 |
| 2 | C | 601 | XEG | OAQ-CAS-OAA | -2.42 | 119.61 | 123.55 |
| 2 | H | 601 | XEG | OAR-CBF-CBE | 2.41 | 115.64 | 109.13 |
| 2 | F | 601 | XEG | CAP-CBE-CBF | 2.41 | 115.08 | 110.16 |
| 2 | A | 601 | XEG | CAM-CAZ-CAS | 2.41 | 124.77 | 120.09 |
| 2 | K | 601 | XEG | CAL-CAZ-CAS | -2.41 | 115.41 | 120.09 |
| 2 | C | 601 | XEG | CAL-CAZ-CAS | -2.39 | 115.43 | 120.09 |
| 2 | E | 601 | XEG | OAR-CBF-CBE | 2.39 | 115.57 | 109.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | E | 601 | XEG | CAP-CBD-CBC | -2.38 | 117.10 | 121.01 |
| 2 | C | 601 | XEG | OAR-CBF-CBE | 2.37 | 115.53 | 109.13 |
| 2 | I | 601 | XEG | CAN-CBC-CBD | -2.37 | 119.41 | 122.06 |
| 2 | B | 601 | XEG | CAP-CBE-CBF | 2.36 | 114.98 | 110.16 |
| 2 | F | 601 | XEG | OAR-CBF-CBE | 2.36 | 115.48 | 109.13 |
| 2 | B | 601 | XEG | CAP-CBD-CBC | -2.35 | 117.15 | 121.01 |
| 2 | J | 601 | XEG | OAR-CBF-CBE | 2.34 | 115.43 | 109.13 |
| 2 | E | 601 | XEG | CAM-CAZ-CAS | 2.33 | 124.63 | 120.09 |
| 2 | G | 601 | XEG | OAQ-CAS-OAA | -2.25 | 119.90 | 123.55 |
| 2 | A | 601 | XEG | CBA-CBF-CBE | -2.23 | 108.16 | 113.70 |
| 2 | L | 601 | XEG | OAR-CBF-CBE | 2.23 | 115.13 | 109.13 |
| 2 | J | 601 | XEG | CAP-CBE-CBF | 2.21 | 114.67 | 110.16 |
| 2 | D | 601 | XEG | OAR-CBF-CBE | 2.20 | 115.05 | 109.13 |
| 2 | C | 601 | XEG | CAN-CBC-CBD | -2.19 | 119.61 | 122.06 |
| 2 | L | 601 | XEG | CAN-CBC-CBD | -2.18 | 119.62 | 122.06 |
| 2 | G | 601 | XEG | CAM-CAZ-CAS | 2.17 | 124.31 | 120.09 |
| 2 | G | 601 | XEG | CAP-CBD-CBC | -2.16 | 117.46 | 121.01 |
| 2 | B | 601 | XEG | CAN-CBC-CBD | -2.16 | 119.64 | 122.06 |
| 2 | F | 601 | XEG | CAL-CAZ-CAS | -2.13 | 115.94 | 120.09 |
| 2 | C | 601 | XEG | CAM-CAZ-CAS | 2.11 | 124.20 | 120.09 |
| 2 | H | 601 | XEG | CAY-CBD-CBC | 2.10 | 119.77 | 117.08 |
| 2 | A | 601 | XEG | CAP-CBD-CBC | -2.09 | 117.58 | 121.01 |
| 2 | H | 601 | XEG | OAQ-CAS-OAA | -2.09 | 120.16 | 123.55 |
| 2 | H | 601 | XEG | CAN-CBC-CBD | -2.08 | 119.73 | 122.06 |
| 2 | K | 601 | XEG | CAM-CAZ-CAS | 2.08 | 124.14 | 120.09 |
| 2 | C | 601 | XEG | CAY-CBD-CBC | 2.07 | 119.74 | 117.08 |
| 2 | F | 601 | XEG | CAN-CBC-CBD | -2.03 | 119.79 | 122.06 |
| 2 | F | 601 | XEG | CAM-CAZ-CAS | 2.02 | 124.02 | 120.09 |
| 2 | A | 601 | XEG | CAJ-CBA-CAO | 2.01 | 121.07 | 118.74 |
| 2 | K | 601 | XEG | OAQ-CAS-OAA | -2.01 | 120.28 | 123.55 |
| 2 | B | 601 | XEG | CAY-CBD-CBC | 2.01 | 119.65 | 117.08 |
| 2 | F | 601 | XEG | CAY-CBD-CBC | 2.01 | 119.65 | 117.08 |

There are no chirality outliers.

All (96) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | A | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | A | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | B | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | B | 601 | XEG | CAZ-CAS-OAQ-CBE |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | C | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | C | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | C | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | D | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | D | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | E | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | E | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | E | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | F | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | F | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | F | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | G | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | G | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | H | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | H | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | I | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | I | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | I | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | J | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | J | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | K | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | K | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | K | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | L | 601 | XEG | OAA-CAS-OAQ-CBE |
| 2 | L | 601 | XEG | CAZ-CAS-OAQ-CBE |
| 2 | L | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | A | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | B | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | D | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | F | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | G | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | I | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | J | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | L | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | H | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | C | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | E | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | H | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | H | 601 | XEG | OAQ-CAS-CAZ-CAM |
| 2 | J | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | K | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | B | 601 | XEG | OAA-CAS-CAZ-CAL |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | D | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | H | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | B | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | D | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | G | 601 | XEG | OAQ-CAS-CAZ-CAL |
| 2 | A | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | B | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | D | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | E | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | F | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | G | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | I | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | J | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | L | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | A | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | C | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | C | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | E | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | F | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | G | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | I | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | J | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | K | 601 | XEG | OAA-CAS-CAZ-CAL |
| 2 | K | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | L | 601 | XEG | OAA-CAS-CAZ-CAM |
| 2 | A | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | C | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | C | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | D | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | F | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | F | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | G | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | G | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | H | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | I | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | I | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | K | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | L | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | B | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | D | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | E | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | A | 601 | XEG | CAO-CBA-CBF-CBE |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | J | 601 | XEG | CAJ-CBA-CBF-CBE |
| 2 | L | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | B | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | E | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | H | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | J | 601 | XEG | CAO-CBA-CBF-CBE |
| 2 | K | 601 | XEG | CAO-CBA-CBF-CBE |

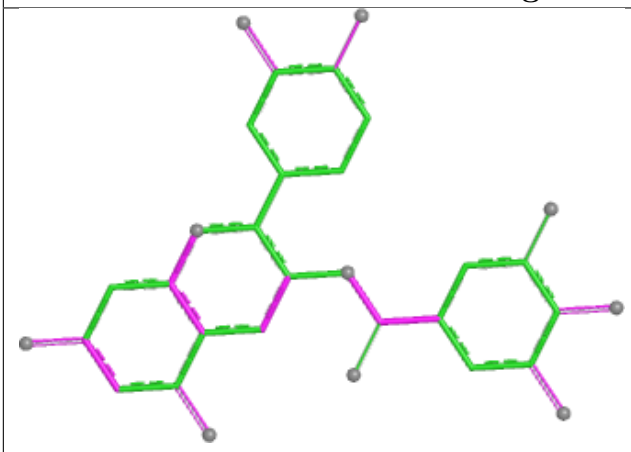
There are no ring outliers.

12 monomers are involved in 36 short contacts:

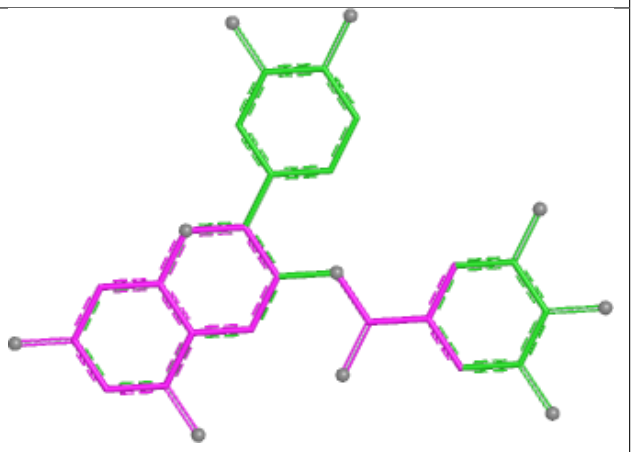
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | C | 601 | XEG | 4 | 0 |
| 2 | E | 601 | XEG | 3 | 0 |
| 2 | G | 601 | XEG | 4 | 0 |
| 2 | I | 601 | XEG | 3 | 0 |
| 2 | F | 601 | XEG | 4 | 0 |
| 2 | B | 601 | XEG | 1 | 0 |
| 2 | J | 601 | XEG | 6 | 0 |
| 2 | A | 601 | XEG | 1 | 0 |
| 2 | D | 601 | XEG | 2 | 0 |
| 2 | L | 601 | XEG | 3 | 0 |
| 2 | H | 601 | XEG | 2 | 0 |
| 2 | K | 601 | XEG | 3 | 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 then 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.

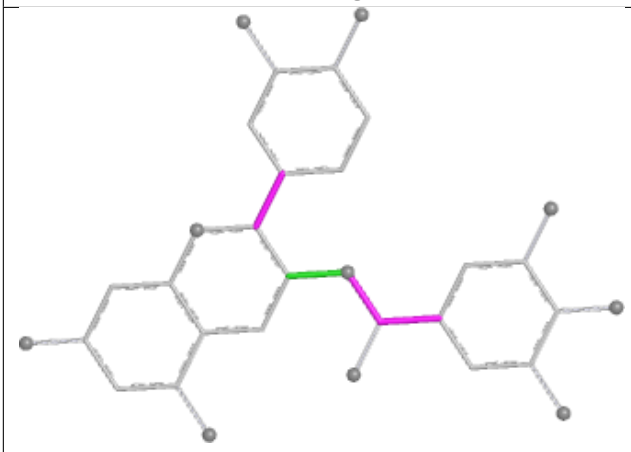
**Ligand XEG C 601**



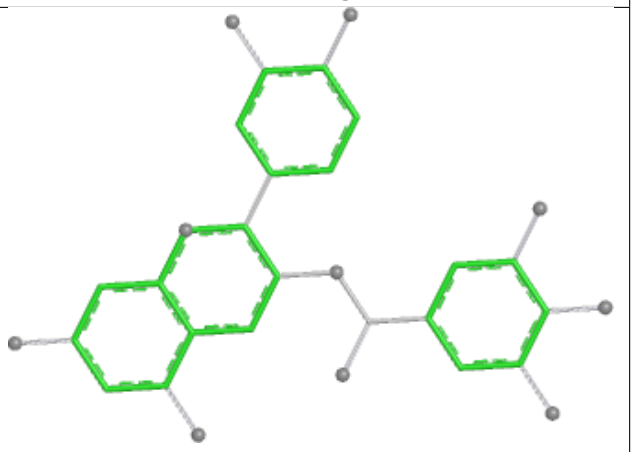
**Bond lengths**



**Bond angles**

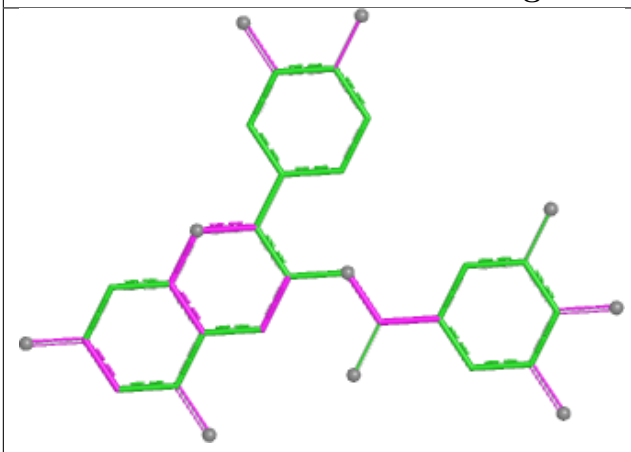


**Torsions**

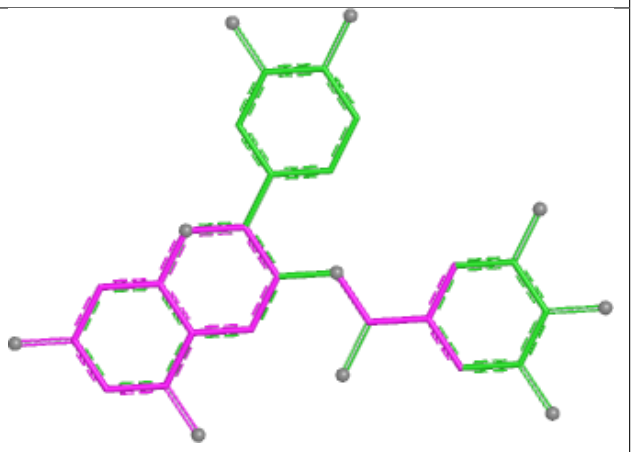


**Rings**

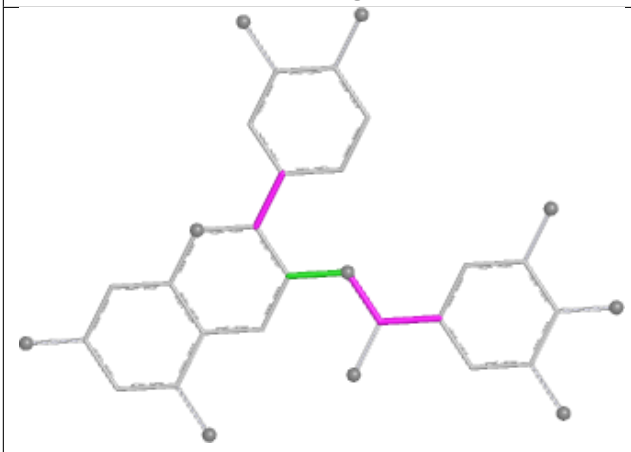
**Ligand XEG E 601**



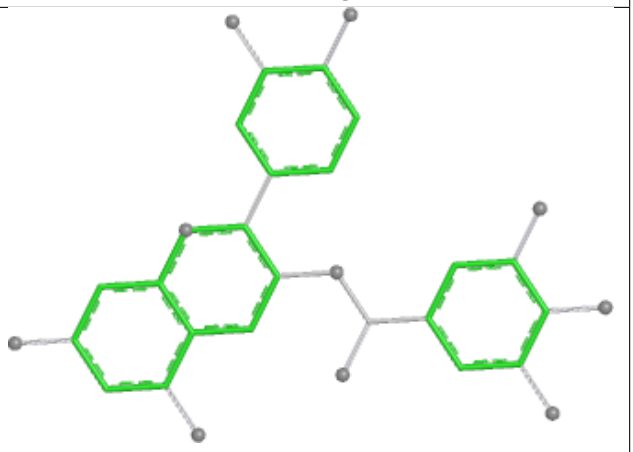
Bond lengths



Bond angles

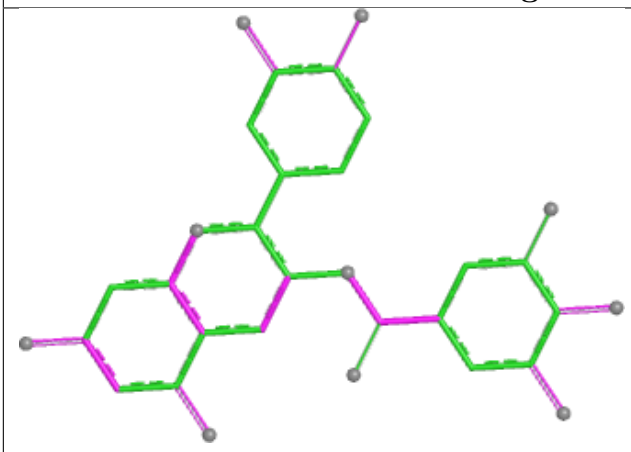


Torsions

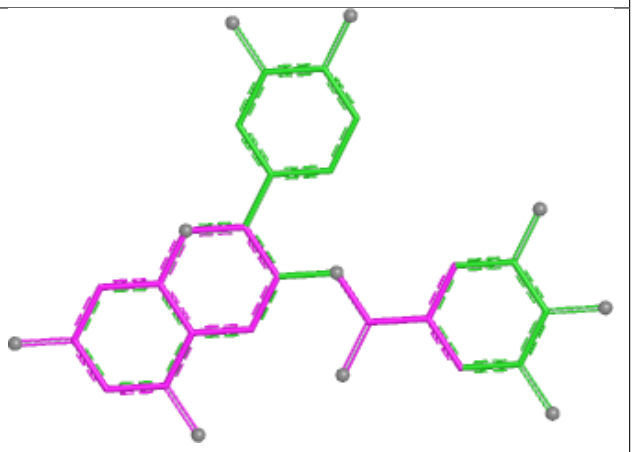


Rings

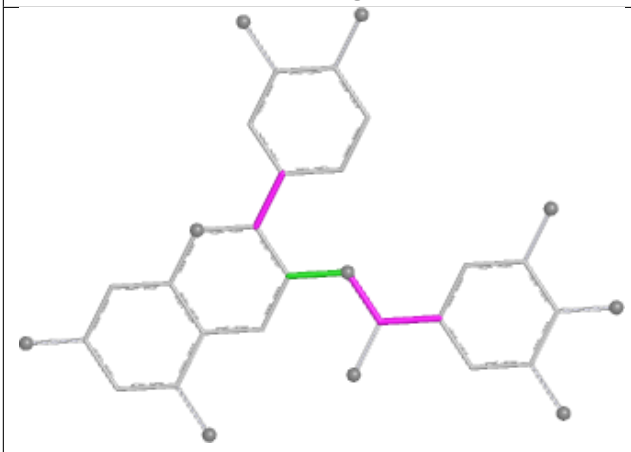
**Ligand XEG G 601**



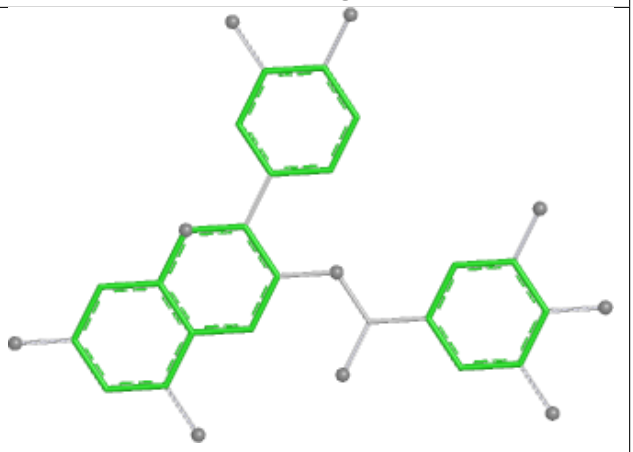
**Bond lengths**



**Bond angles**

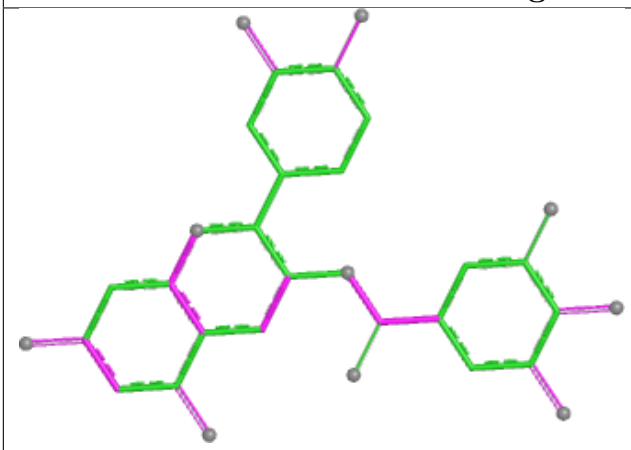


**Torsions**

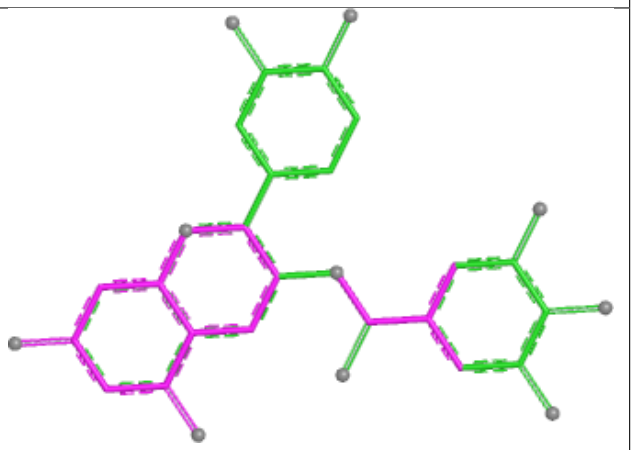


**Rings**

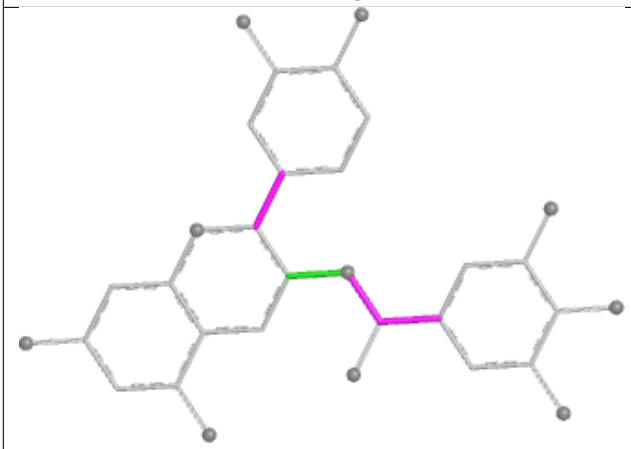
**Ligand XEG I 601**



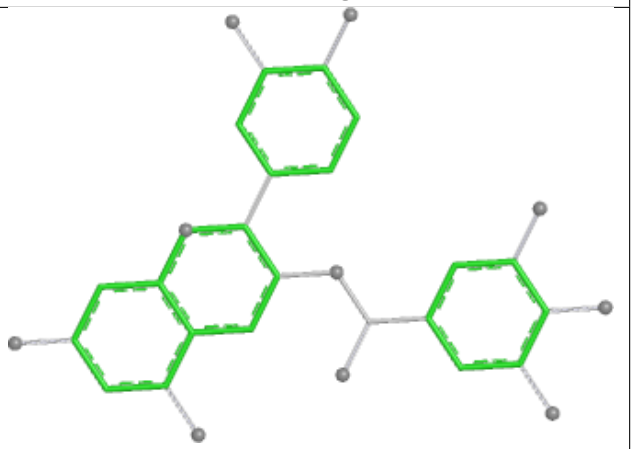
**Bond lengths**



**Bond angles**

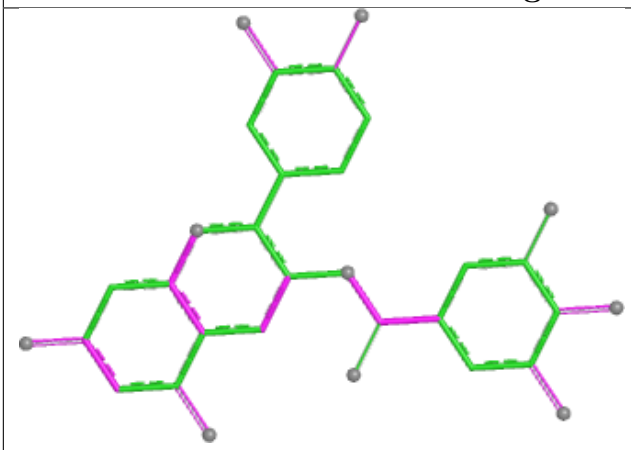


**Torsions**

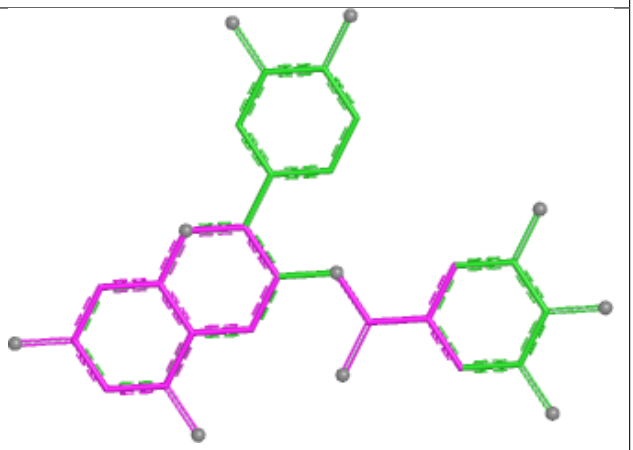


**Rings**

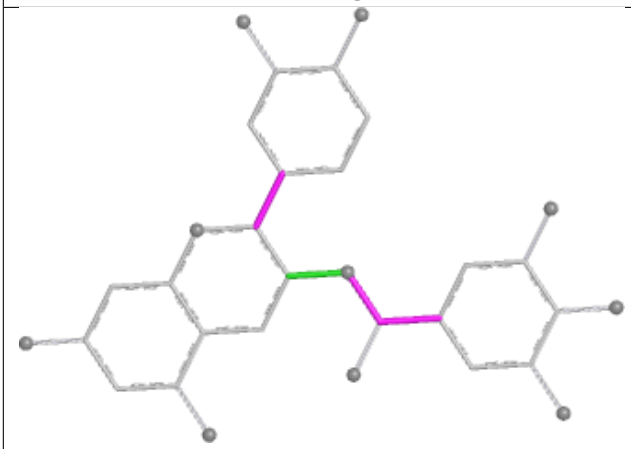
**Ligand XEG F 601**



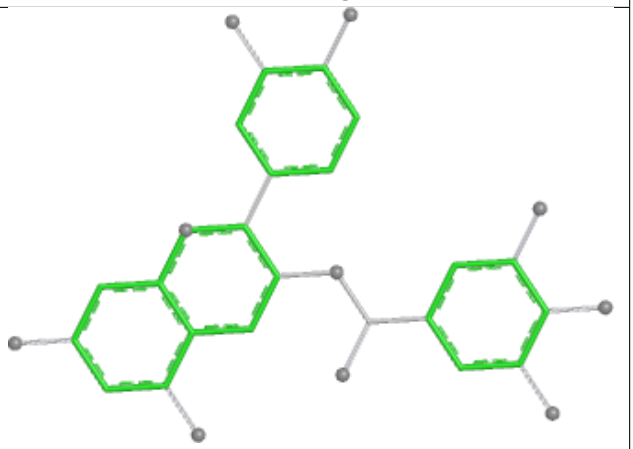
**Bond lengths**



**Bond angles**

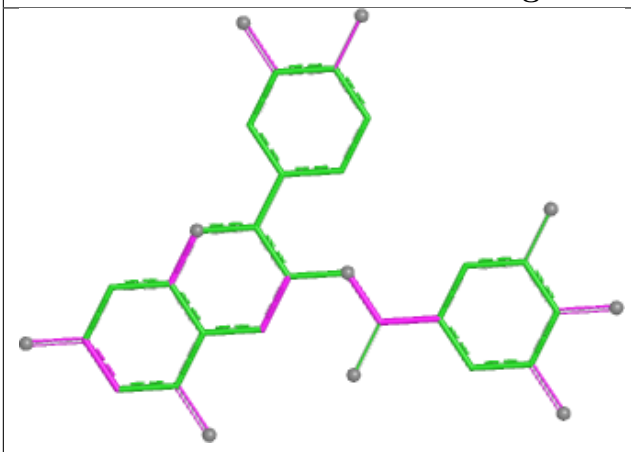


**Torsions**

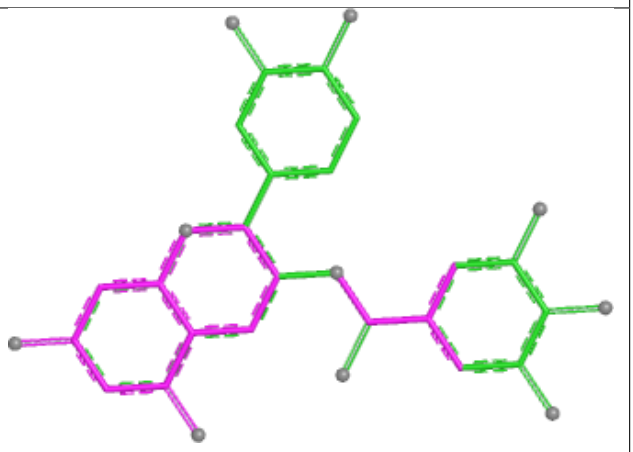


**Rings**

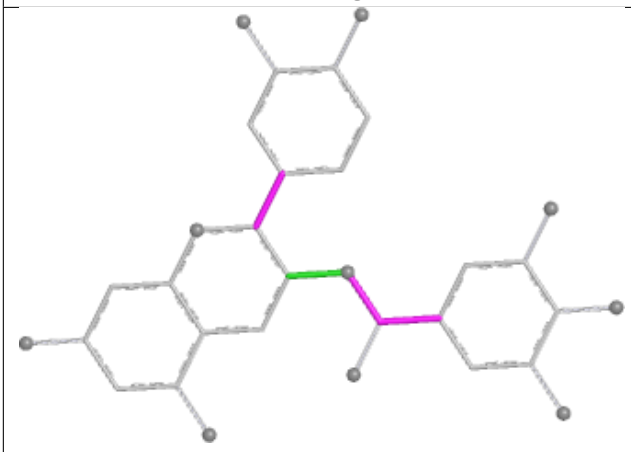
**Ligand XEG B 601**



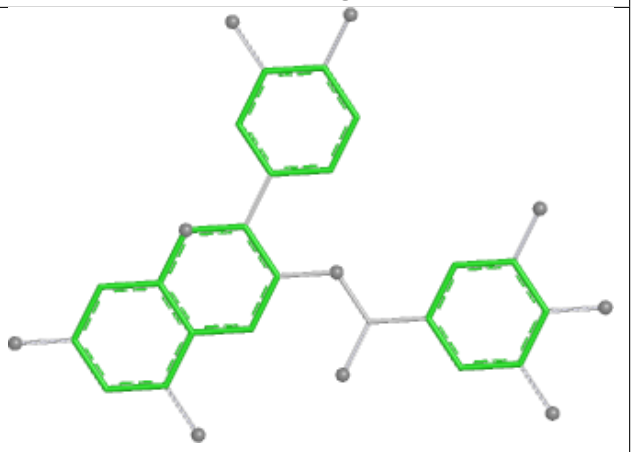
Bond lengths



Bond angles

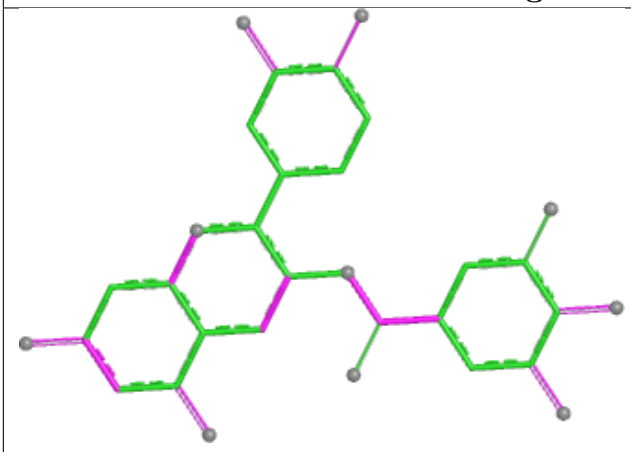


Torsions

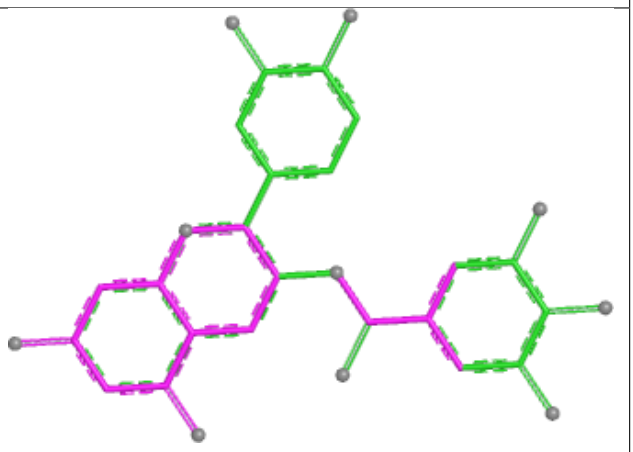


Rings

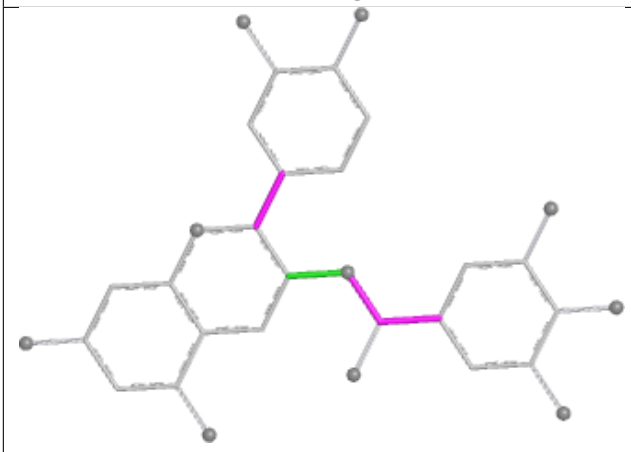
**Ligand XEG J 601**



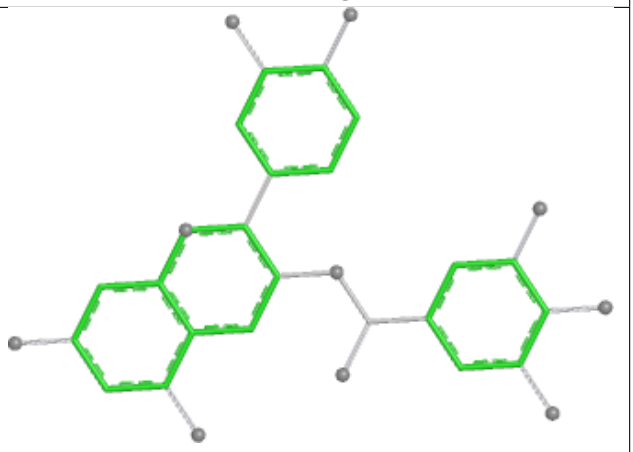
**Bond lengths**



**Bond angles**

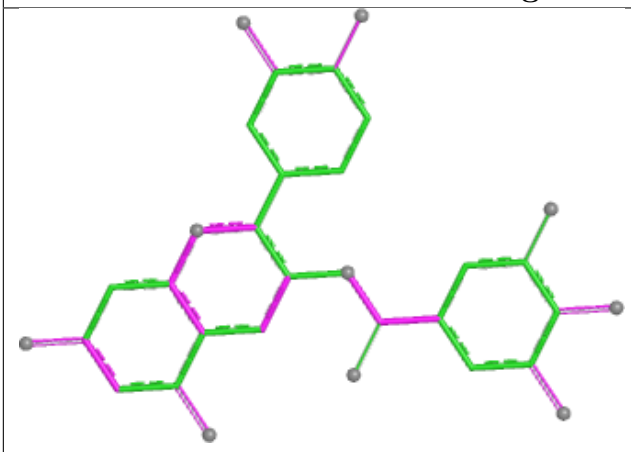


**Torsions**

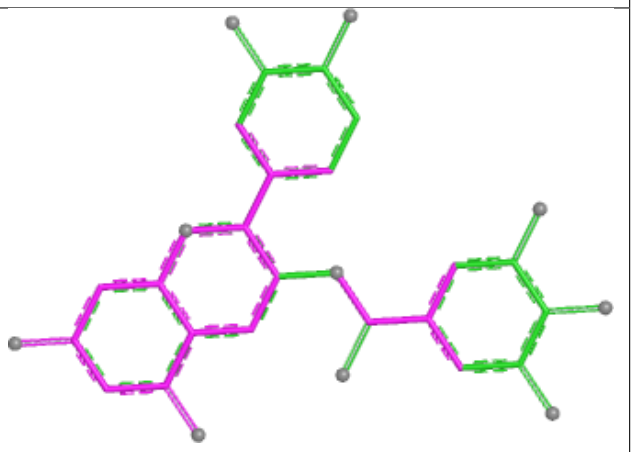


**Rings**

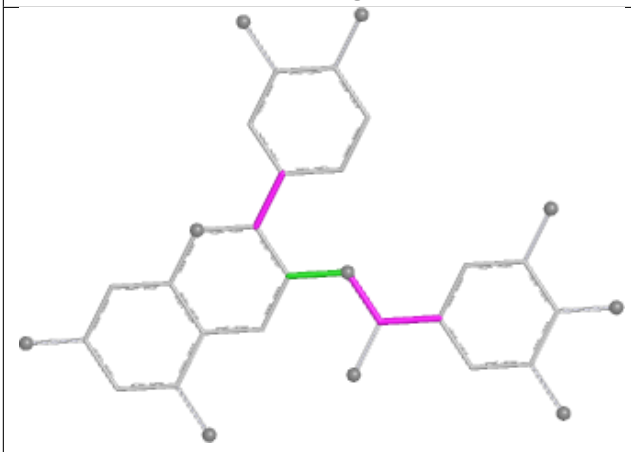
**Ligand XEG A 601**



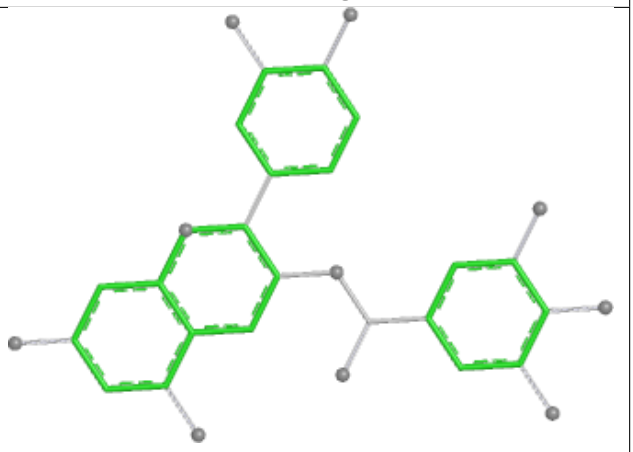
**Bond lengths**



**Bond angles**

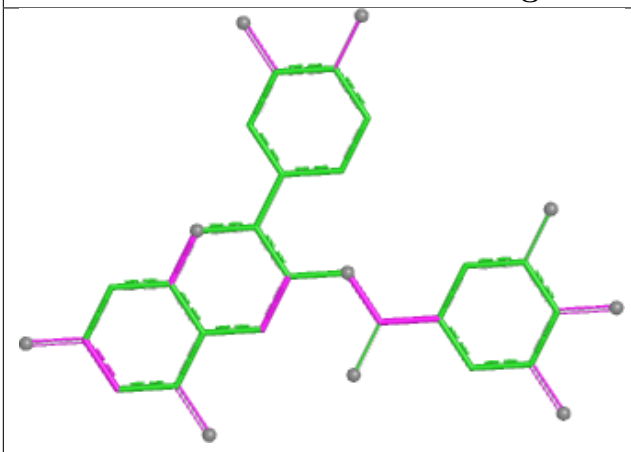


**Torsions**

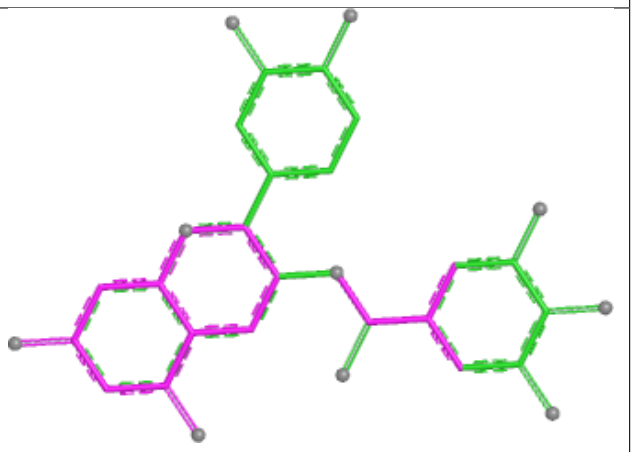


**Rings**

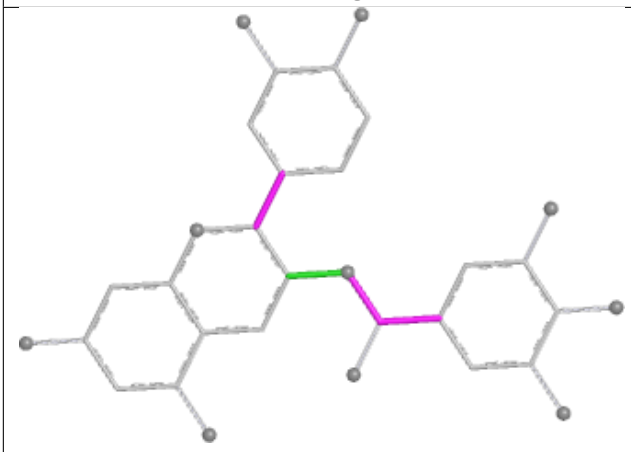
**Ligand XEG D 601**



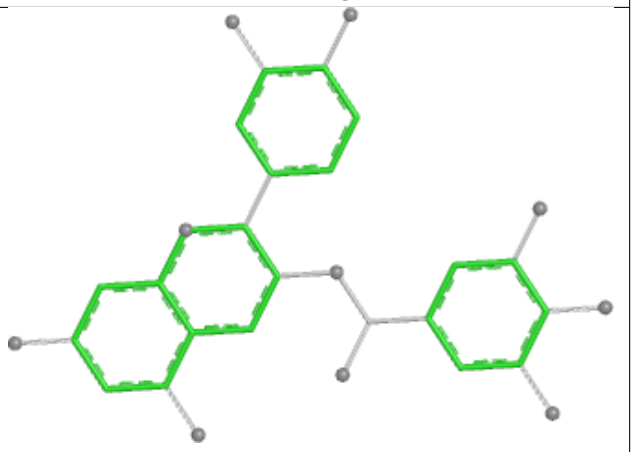
**Bond lengths**



**Bond angles**

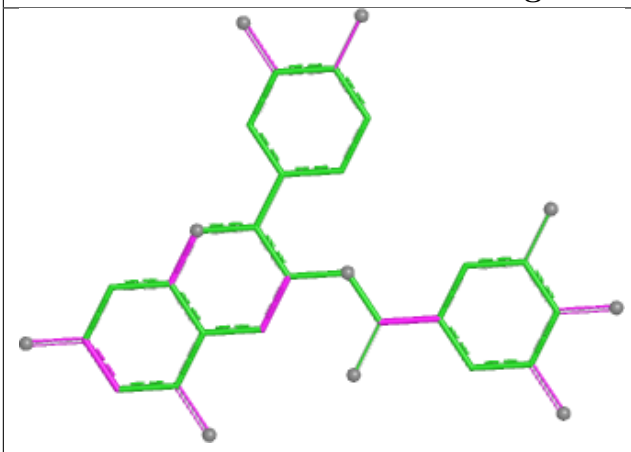


**Torsions**

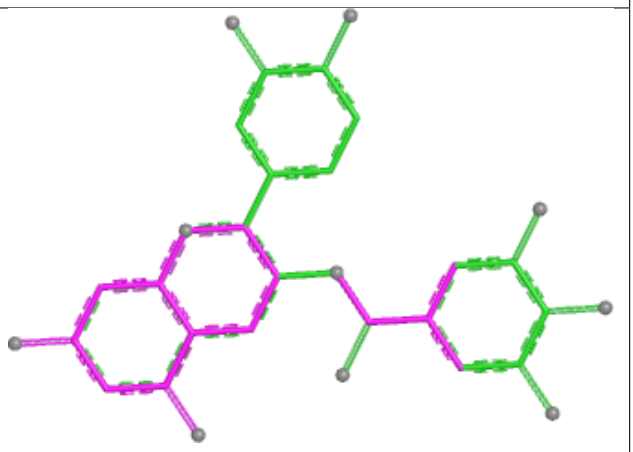


**Rings**

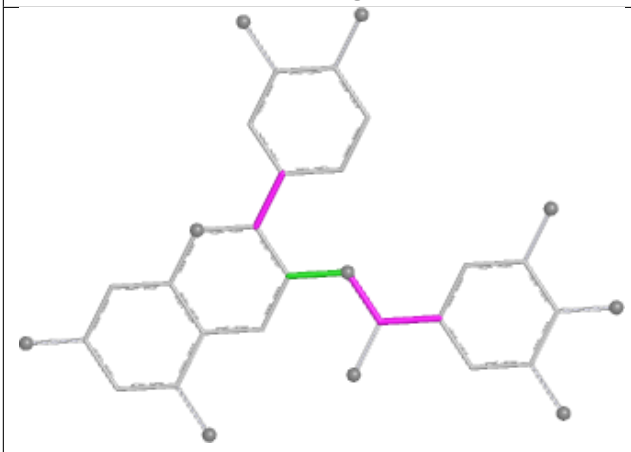
**Ligand XEG L 601**



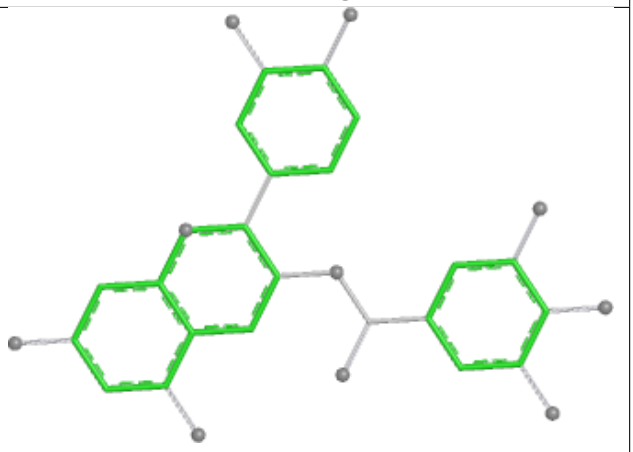
**Bond lengths**



**Bond angles**

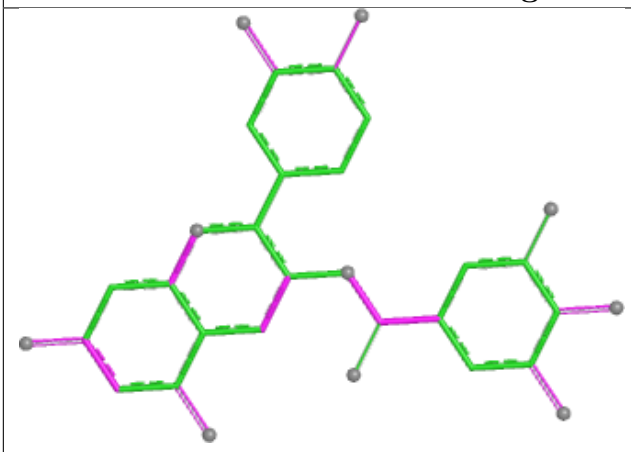


**Torsions**

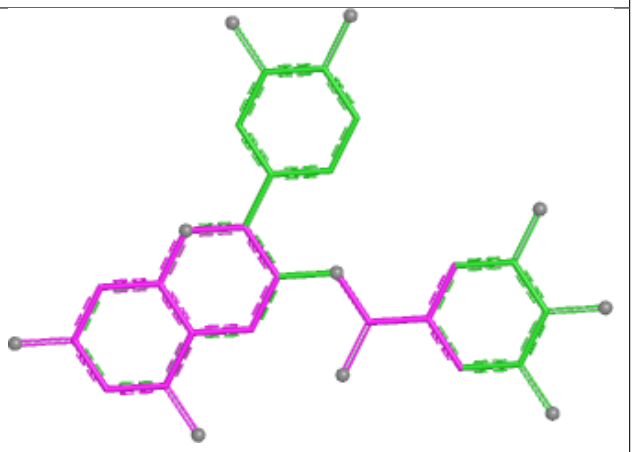


**Rings**

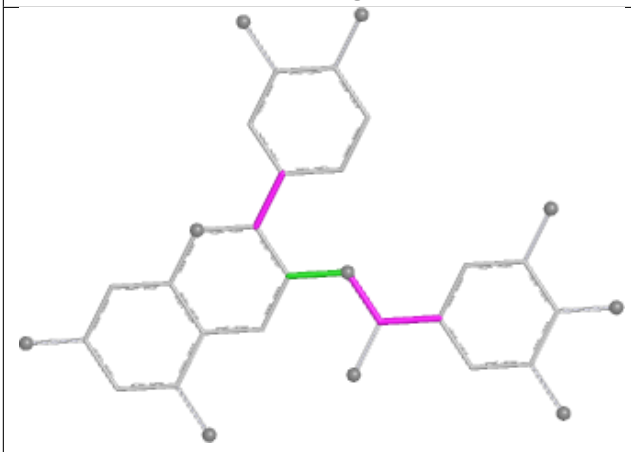
**Ligand XEG H 601**



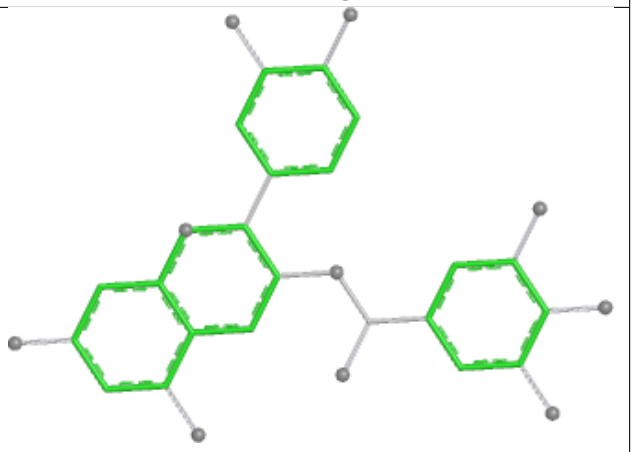
**Bond lengths**



**Bond angles**

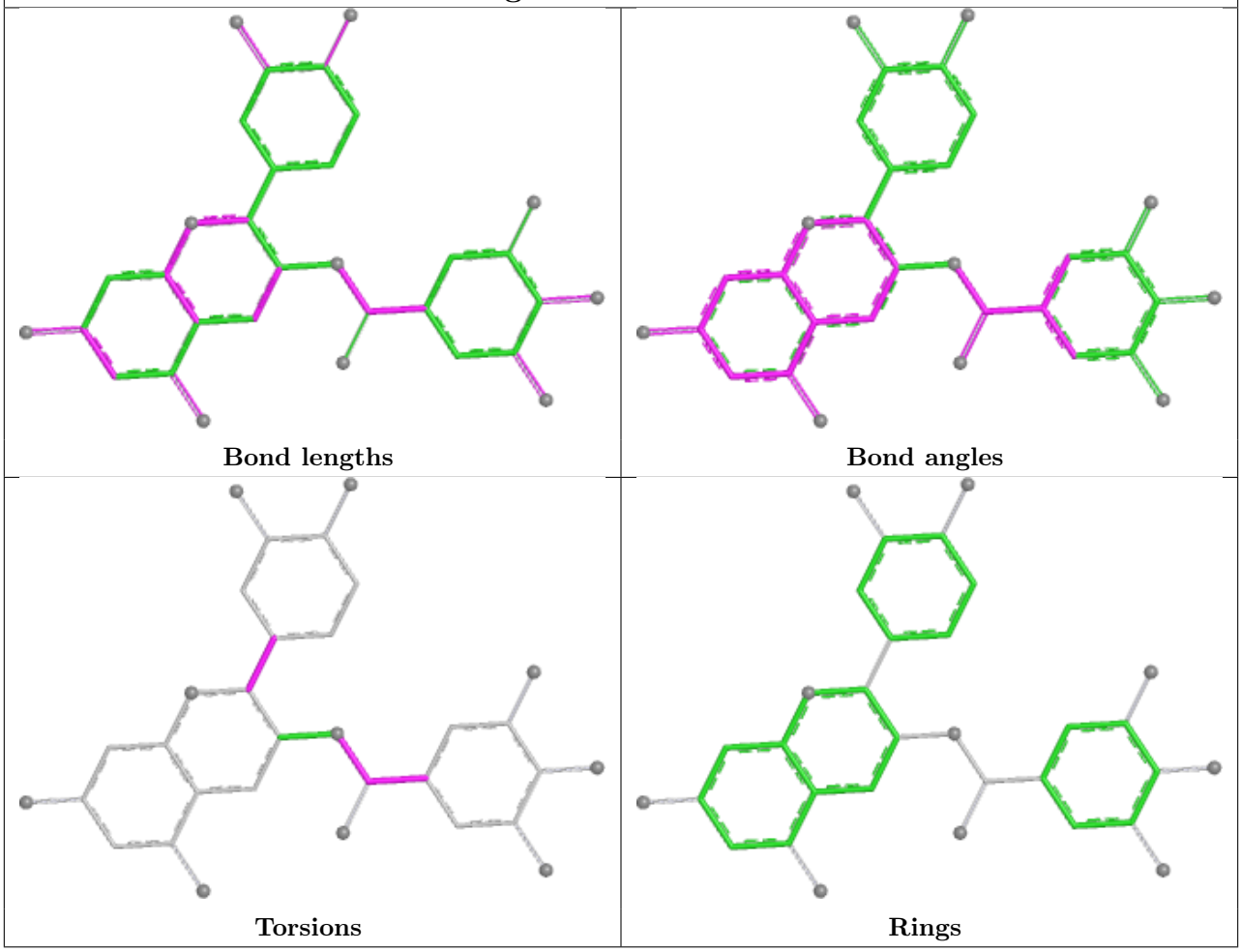


**Torsions**



**Rings**

**Ligand XEG K 601**




## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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, $95^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 496/496 (100%) | -1.08 | 0 100 100 | 66, 125, 228, 270 | 0 |
| 1 | B | 496/496 (100%) | -1.14 | 0 100 100 | 69, 119, 220, 268 | 0 |
| 1 | C | 496/496 (100%) | -1.03 | 1 (0%) 91 79 | 61, 119, 224, 266 | 0 |
| 1 | D | 496/496 (100%) | -1.13 | 1 (0%) 91 79 | 66, 119, 222, 275 | 0 |
| 1 | E | 496/496 (100%) | -1.10 | 0 100 100 | 66, 126, 228, 269 | 0 |
| 1 | F | 496/496 (100%) | -1.07 | 1 (0%) 91 79 | 60, 120, 228, 267 | 0 |
| 1 | G | 496/496 (100%) | -1.16 | 1 (0%) 91 79 | 58, 112, 219, 277 | 0 |
| 1 | H | 496/496 (100%) | -1.10 | 0 100 100 | 60, 105, 201, 251 | 0 |
| 1 | I | 496/496 (100%) | -1.12 | 2 (0%) 88 71 | 58, 112, 218, 261 | 0 |
| 1 | J | 496/496 (100%) | -1.18 | 0 100 100 | 63, 106, 203, 251 | 0 |
| 1 | K | 496/496 (100%) | -1.10 | 0 100 100 | 61, 114, 221, 276 | 0 |
| 1 | L | 496/496 (100%) | -1.12 | 1 (0%) 91 79 | 60, 114, 215, 265 | 0 |
| All | All | 5952/5952 (100%) | -1.11 | 7 (0%) 92 86 | 58, 116, 222, 277 | 0 |

All (7) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | I | 6 | ASP | 4.1 |
| 1 | C | 227 | ILE | 3.9 |
| 1 | D | 283 | PRO | 2.6 |
| 1 | L | 312 | GLY | 2.2 |
| 1 | I | 355 | GLU | 2.1 |
| 1 | G | 312 | GLY | 2.1 |
| 1 | F | 227 | ILE | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 6.4 Ligands (i)

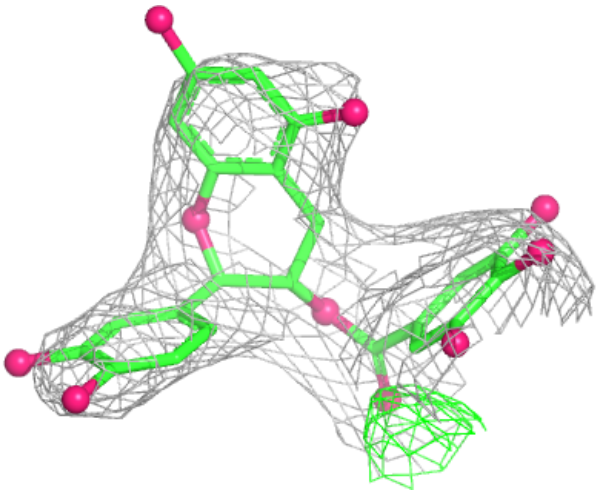
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

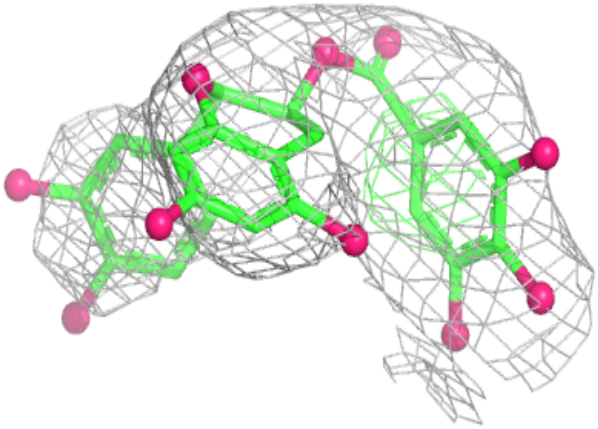
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | XEG | E | 601 | 32/32 | 0.96 | 0.06 | 90,108,125,127 | 0 |
| 2 | XEG | A | 601 | 32/32 | 0.97 | 0.05 | 88,106,122,127 | 0 |
| 2 | XEG | L | 601 | 32/32 | 0.97 | 0.07 | 89,117,128,133 | 0 |
| 2 | XEG | C | 601 | 32/32 | 0.98 | 0.07 | 96,116,133,138 | 0 |
| 2 | XEG | F | 601 | 32/32 | 0.98 | 0.04 | 98,118,134,139 | 0 |
| 2 | XEG | G | 601 | 32/32 | 0.98 | 0.06 | 93,112,124,132 | 0 |
| 2 | XEG | I | 601 | 32/32 | 0.98 | 0.04 | 92,115,127,130 | 0 |
| 2 | XEG | K | 601 | 32/32 | 0.98 | 0.04 | 89,111,123,126 | 0 |
| 2 | XEG | D | 601 | 32/32 | 0.98 | 0.05 | 86,110,123,129 | 0 |
| 2 | XEG | J | 601 | 32/32 | 0.99 | 0.04 | 85,110,122,128 | 0 |
| 2 | XEG | H | 601 | 32/32 | 0.99 | 0.05 | 85,108,121,126 | 0 |
| 2 | XEG | B | 601 | 32/32 | 0.99 | 0.04 | 89,110,125,128 | 0 |

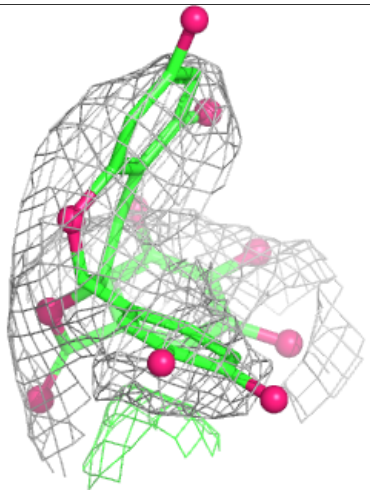
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around XEG E 601:**

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

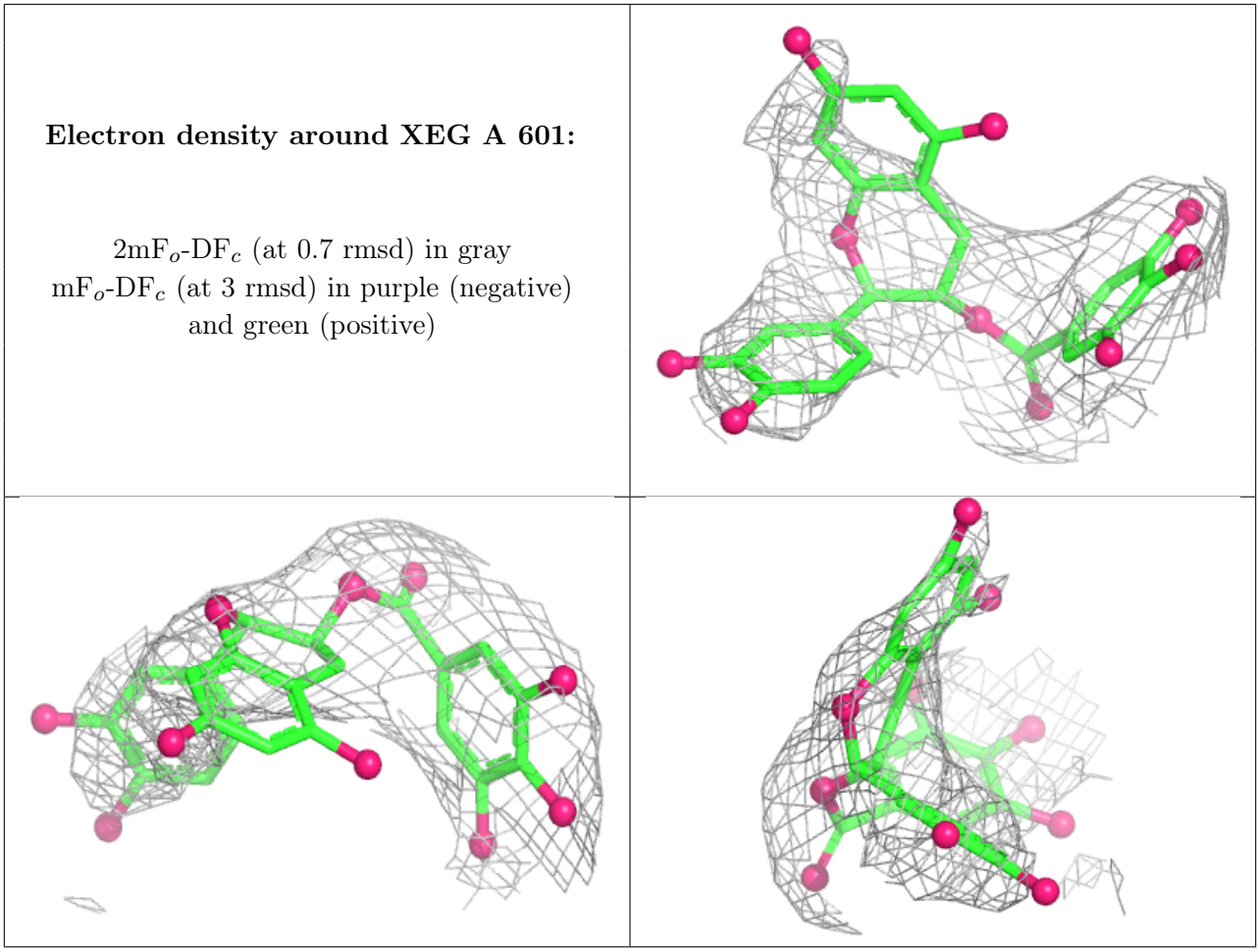






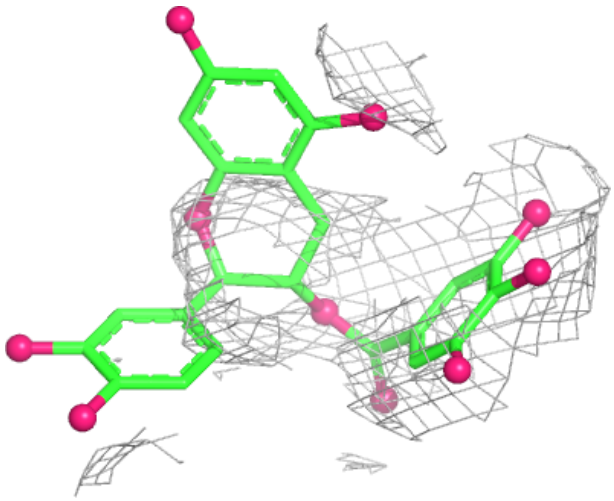
**Electron density around XEG A 601:**

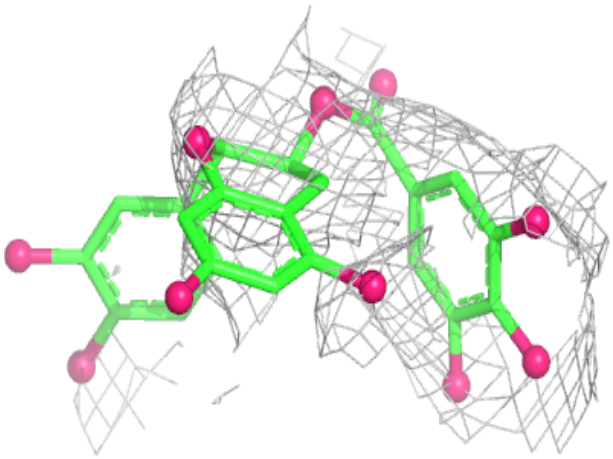
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

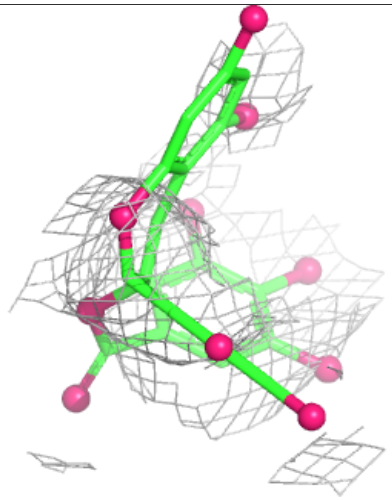


**Electron density around XEG L 601:**

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

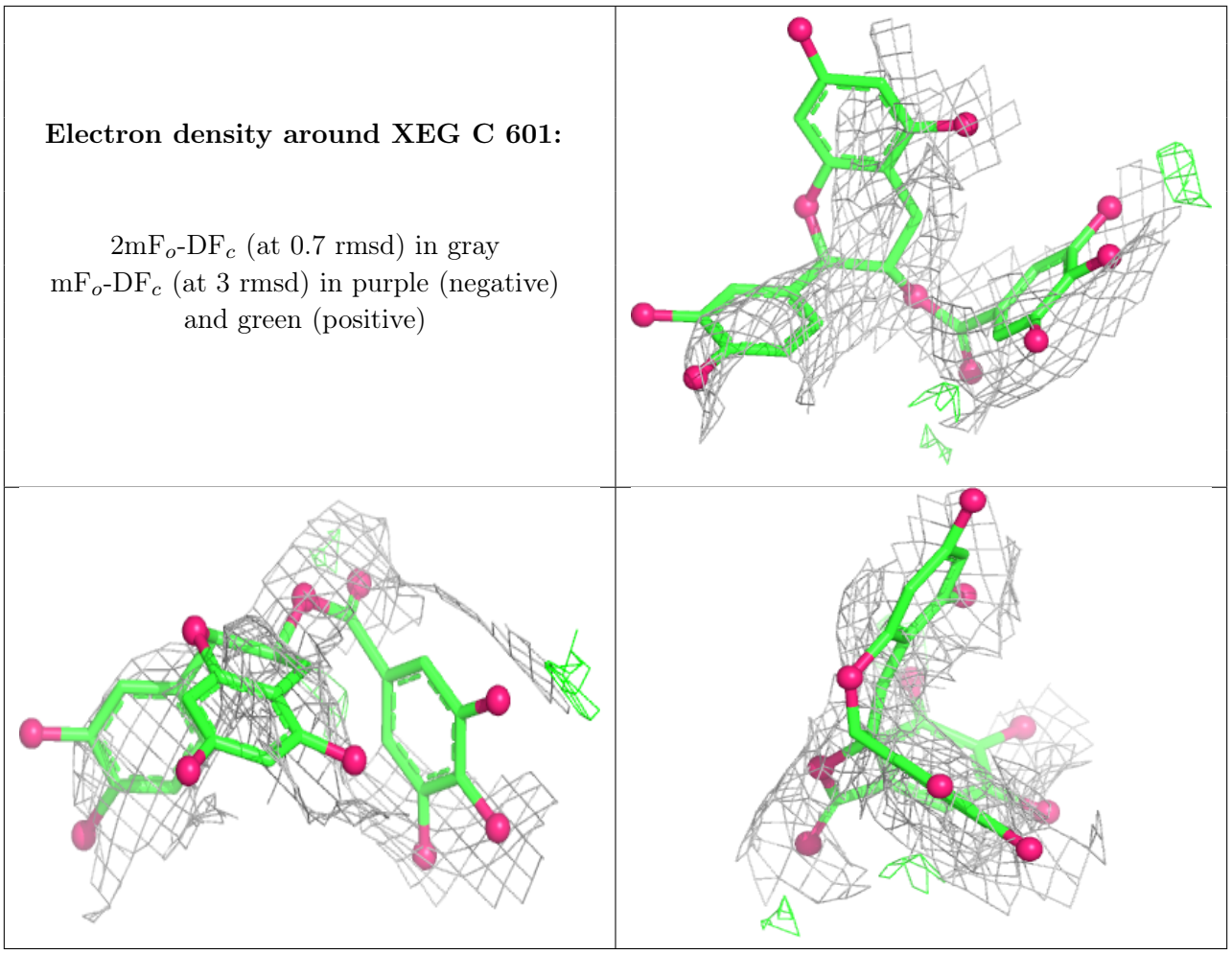






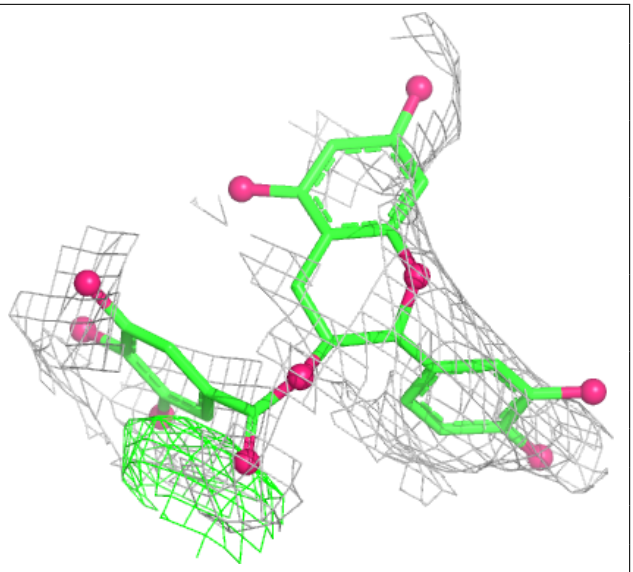
**Electron density around XEG C 601:**

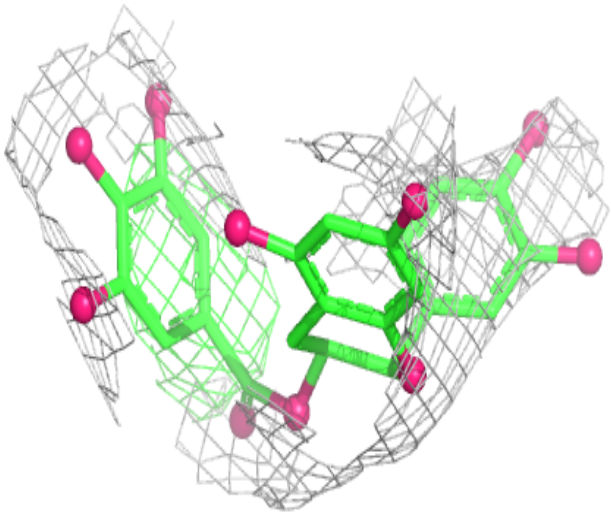
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

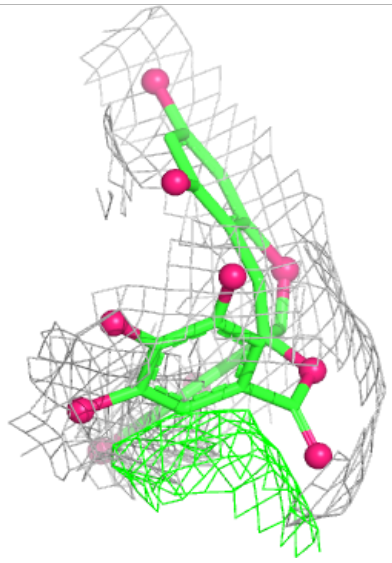


**Electron density around XEG F 601:**

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

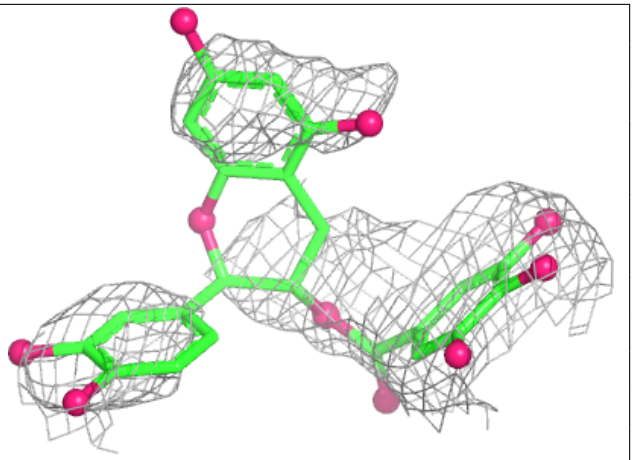


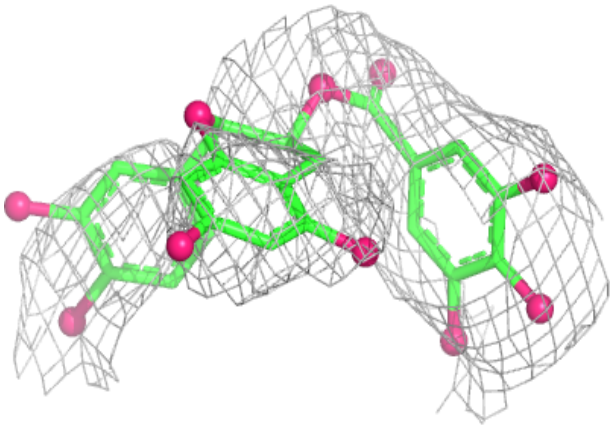


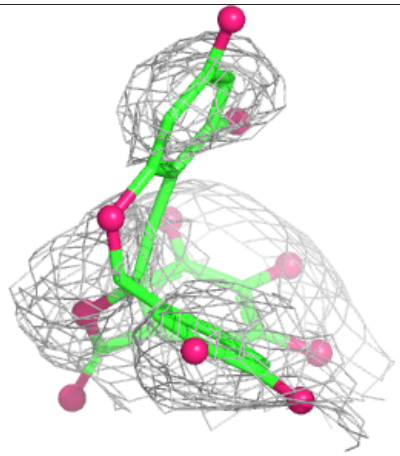


**Electron density around XEG G 601:**

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

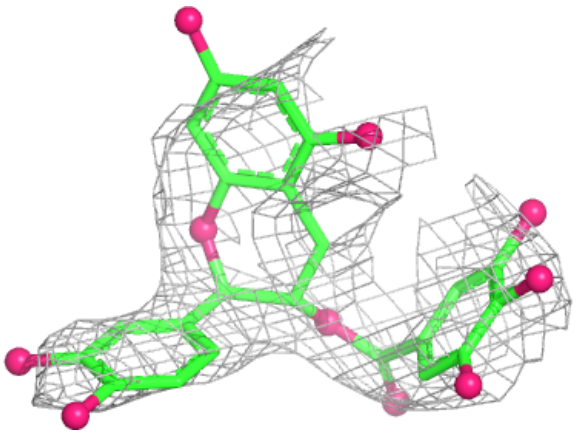


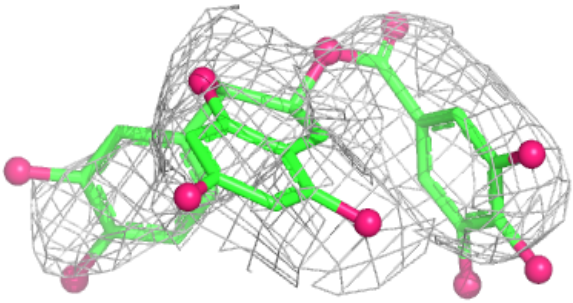


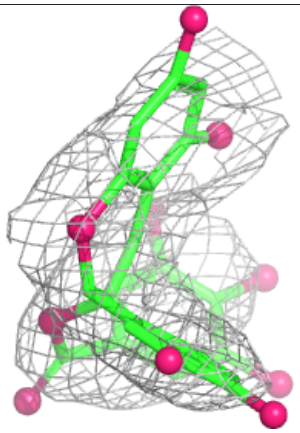


**Electron density around XEG I 601:**

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

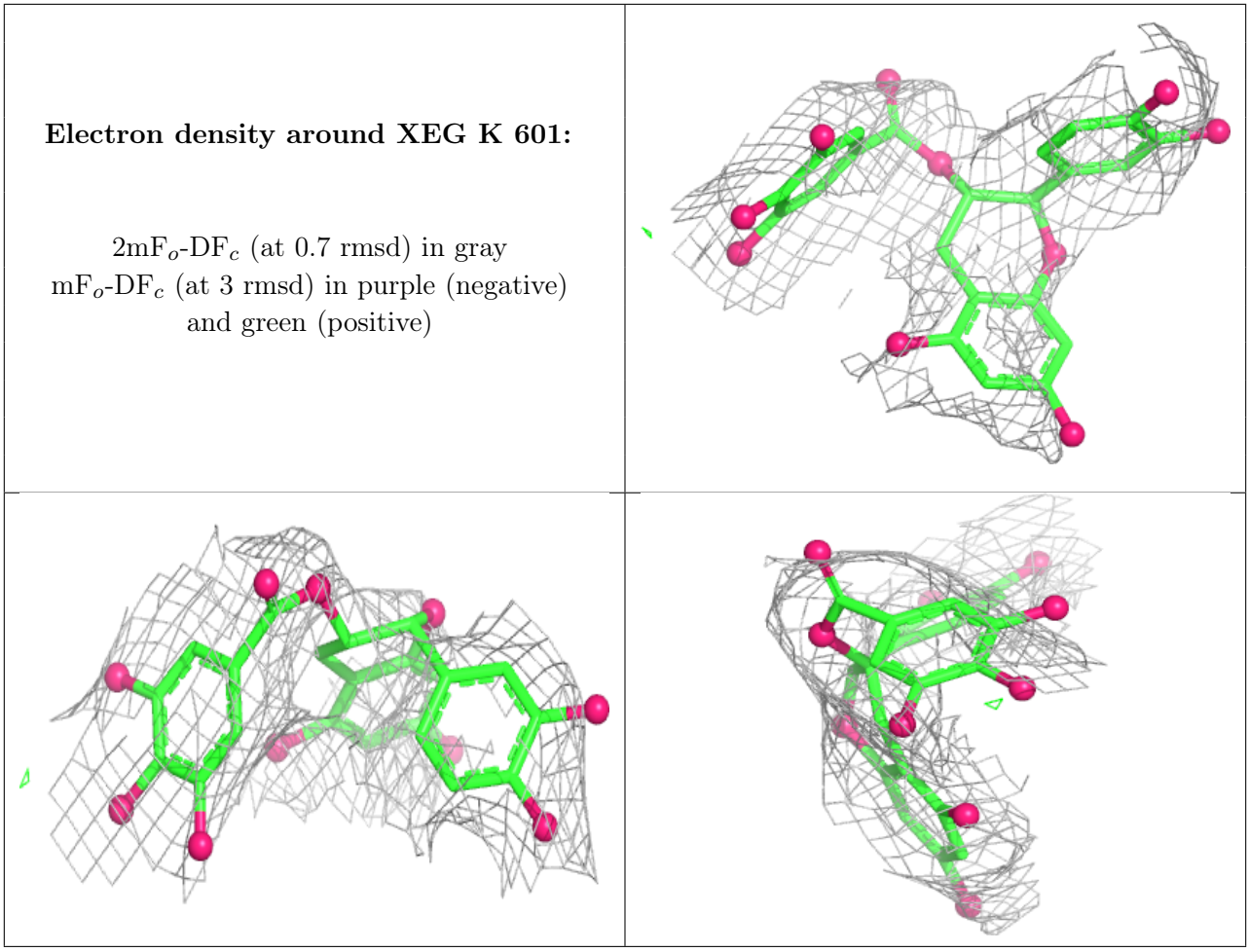






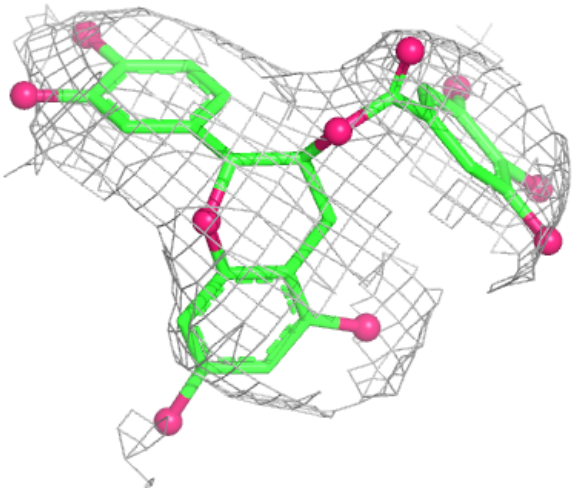
**Electron density around XEG K 601:**

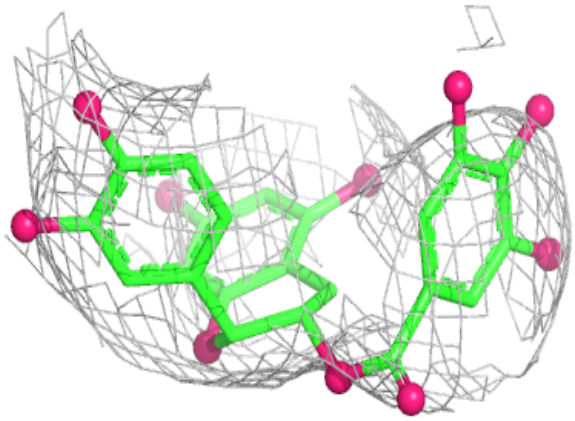
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

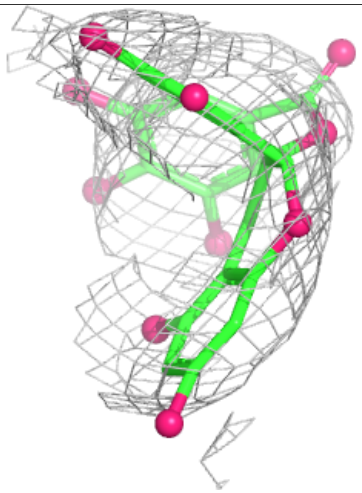


**Electron density around XEG D 601:**

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

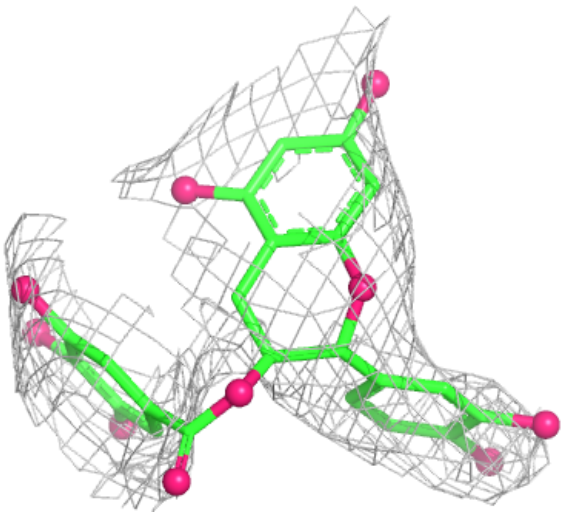


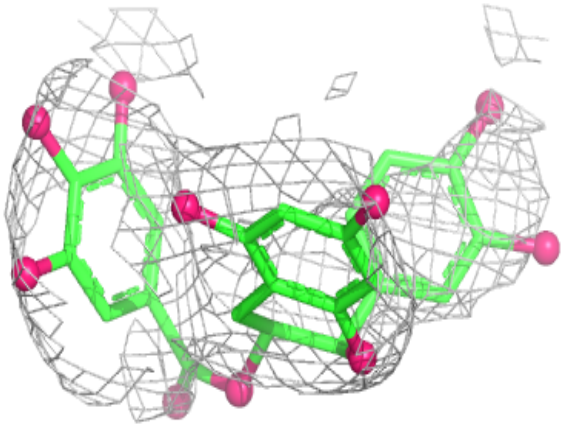


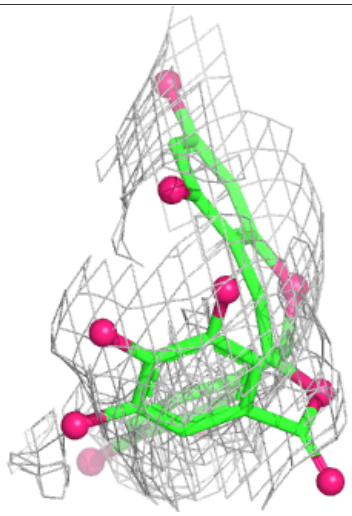


**Electron density around XEG J 601:**

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

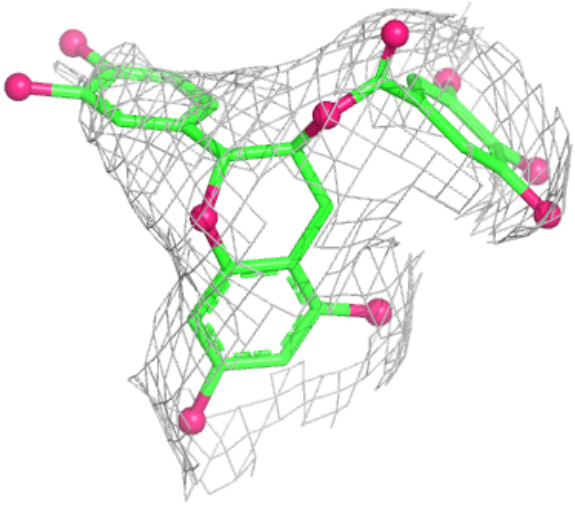


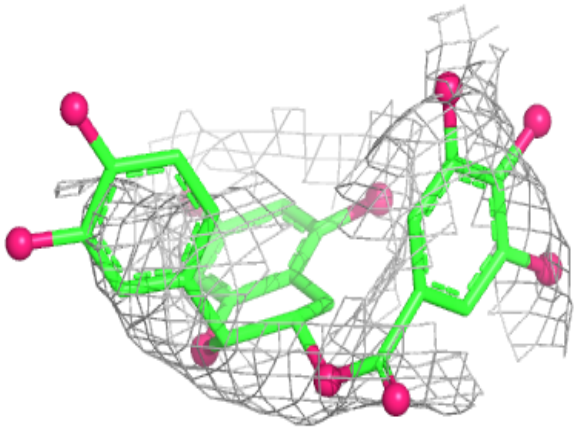


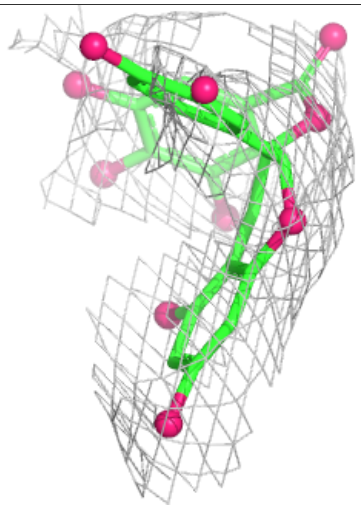


**Electron density around XEG H 601:**

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

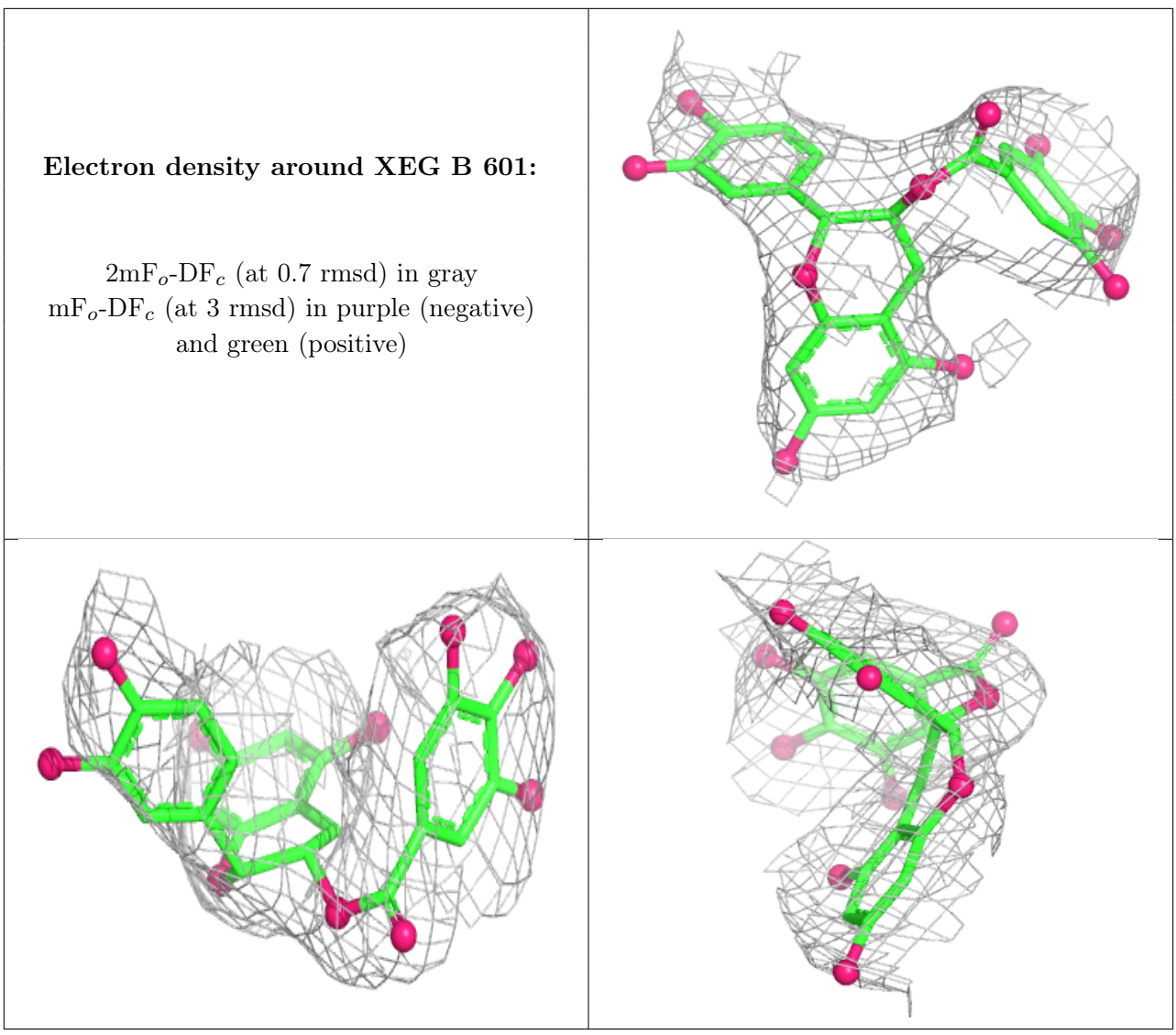






**Electron density around XEG B 601:**

$2mF_o$-$DF_c$ (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.