



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:41 AM GMT

PDB ID : 1SOJ
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B IN COMPLEX WITH IBMX
Authors : Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.
Deposited on : 2004-03-15
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

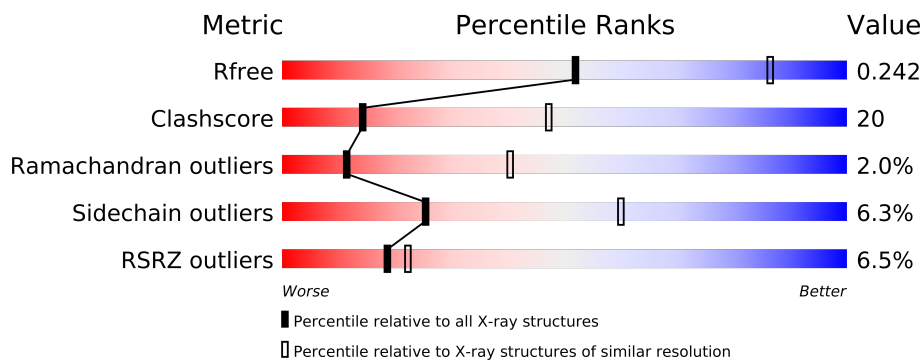
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1053 (2.90-2.90) |
| Clashscore | 79885 | 1326 (2.90-2.90) |
| Ramachandran outliers | 78287 | 1290 (2.90-2.90) |
| Sidechain outliers | 78261 | 1292 (2.90-2.90) |
| RSRZ outliers | 66119 | 1054 (2.90-2.90) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 420 | |
| 1 | B | 420 | |
| 1 | C | 420 | |
| 1 | D | 420 | |
| 1 | E | 420 | |
| 1 | F | 420 | |
| 1 | G | 420 | |
| 1 | H | 420 | |
| 1 | I | 420 | |
| 1 | J | 420 | |
| 1 | K | 420 | |
| 1 | L | 420 | |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36048 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 364 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2907 | 1862 | 496 | 535 | 14 | | | |
| 1 | B | 381 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3017 | 1922 | 519 | 562 | 14 | | | |
| 1 | C | 364 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2907 | 1862 | 496 | 535 | 14 | | | |
| 1 | D | 381 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3017 | 1922 | 519 | 562 | 14 | | | |
| 1 | E | 364 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2907 | 1862 | 496 | 535 | 14 | | | |
| 1 | F | 381 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3017 | 1922 | 519 | 562 | 14 | | | |
| 1 | G | 364 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2907 | 1862 | 496 | 535 | 14 | | | |
| 1 | H | 381 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3017 | 1922 | 519 | 562 | 14 | | | |
| 1 | I | 364 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2907 | 1862 | 496 | 535 | 14 | | | |
| 1 | J | 381 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3017 | 1922 | 519 | 562 | 14 | | | |
| 1 | K | 364 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2907 | 1862 | 496 | 535 | 14 | | | |
| 1 | L | 381 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3017 | 1922 | 519 | 562 | 14 | | | |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | G | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 2 | J | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2 | D | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | K | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | E | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | H | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | B | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | I | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | C | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | A | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | L | 2 | Total 2 | Mg 2 | 0 | 0 |
| 2 | F | 2 | Total 2 | Mg 2 | 0 | 0 |

- Molecule 3 is 3-ISOBUTYL-1-METHYLBXANTHINE (three-letter code: IBM) (formula: $C_{10}H_{14}N_4O_2$).

Image for chem-comp IBM is not available.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 3 | A | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |
| 3 | B | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |
| 3 | C | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |
| 3 | D | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |
| 3 | E | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |
| 3 | F | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |
| 3 | G | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |
| 3 | H | 1 | Total 16 | C 10 | N 4 | O 2 | 0 | 0 |

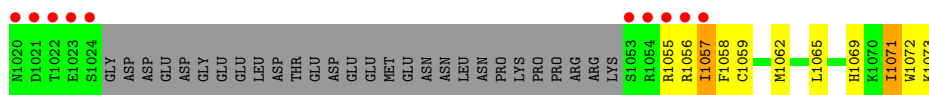
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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3 | I | 1 | Total | C | N | O | 0 | 0 |
| | | | 16 | 10 | 4 | 2 | | |
| 3 | J | 1 | Total | C | N | O | 0 | 0 |
| | | | 16 | 10 | 4 | 2 | | |
| 3 | K | 1 | Total | C | N | O | 0 | 0 |
| | | | 16 | 10 | 4 | 2 | | |
| 3 | L | 1 | Total | C | N | O | 0 | 0 |
| | | | 16 | 10 | 4 | 2 | | |

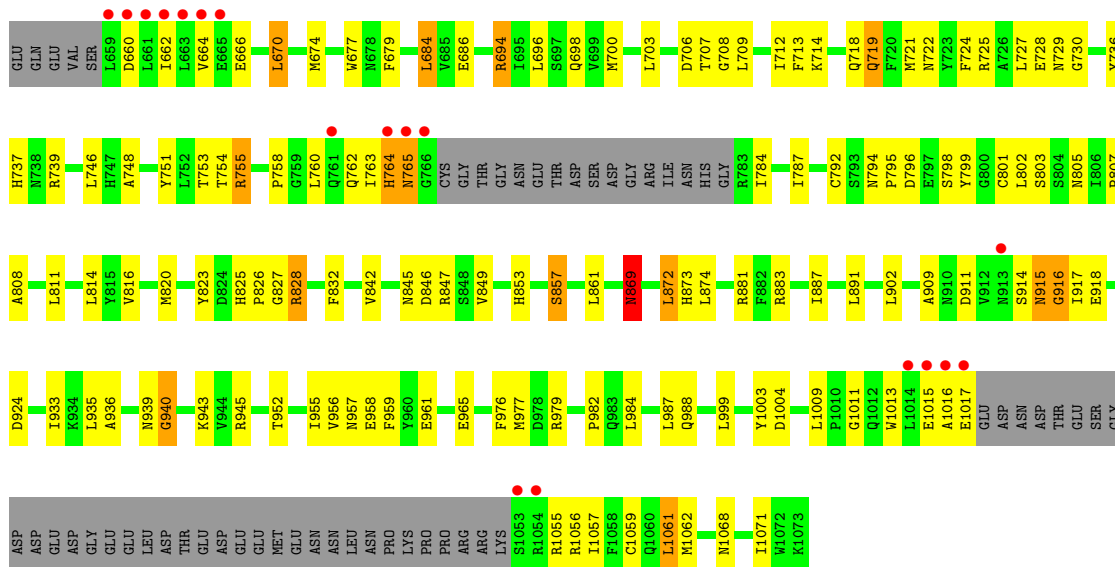
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | A | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 4 | B | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 4 | C | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 4 | D | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 4 | E | 23 | Total | O | 0 | 0 |
| | | | 23 | 23 | | |
| 4 | F | 25 | Total | O | 0 | 0 |
| | | | 25 | 25 | | |
| 4 | G | 23 | Total | O | 0 | 0 |
| | | | 23 | 23 | | |
| 4 | H | 25 | Total | O | 0 | 0 |
| | | | 25 | 25 | | |
| 4 | I | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 4 | J | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 4 | K | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 4 | L | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |



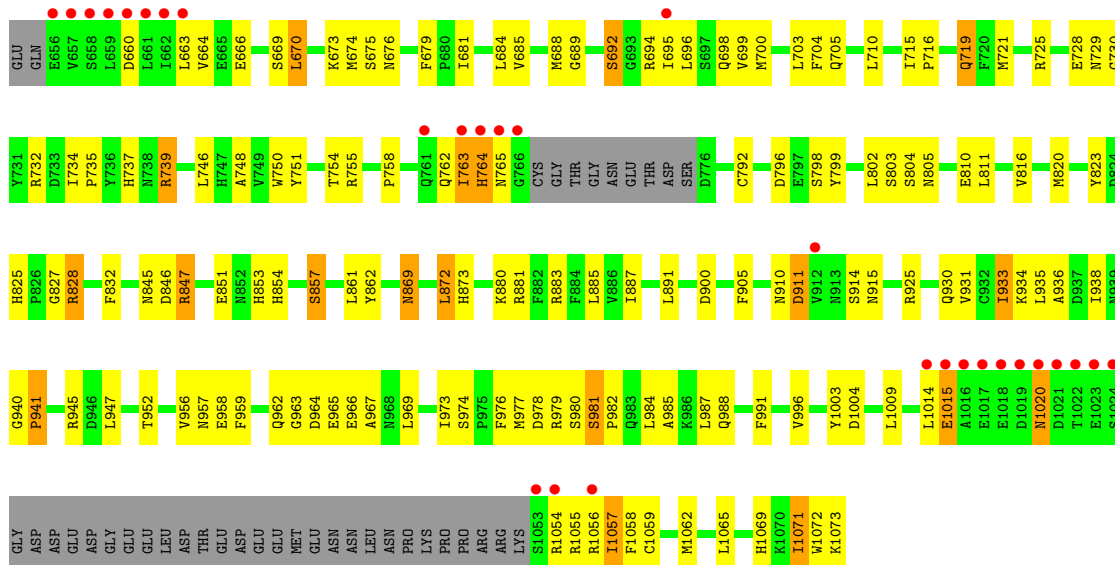
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

Chain C:



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

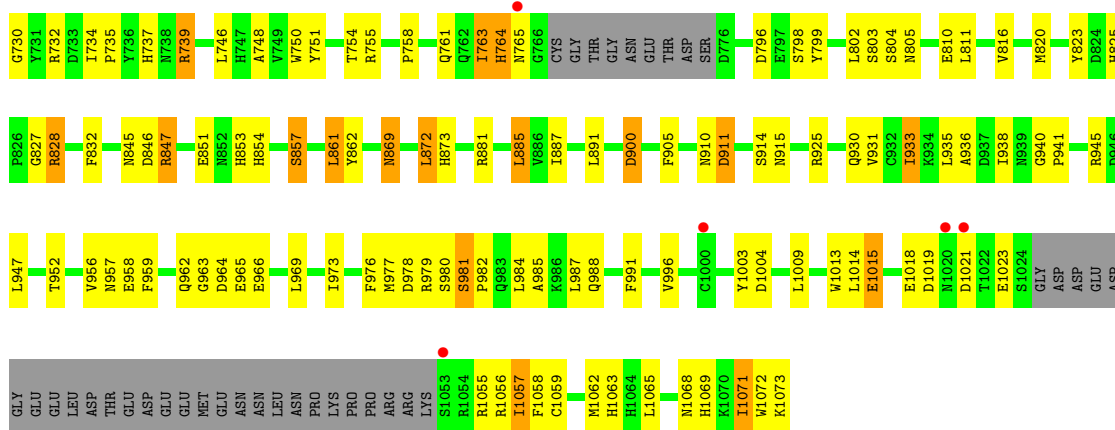
Chain D:



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

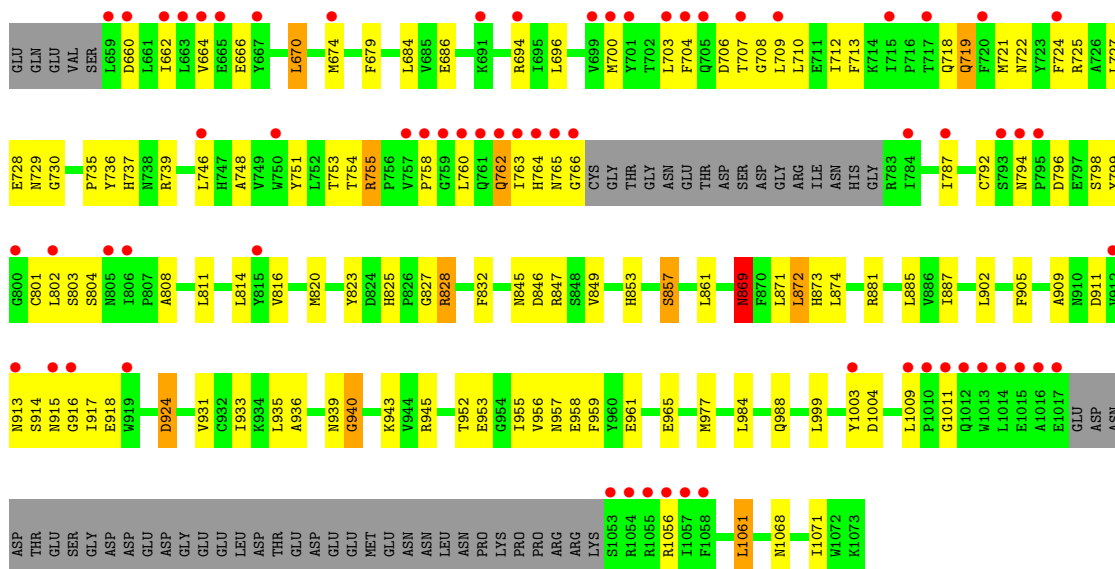
Chain E:





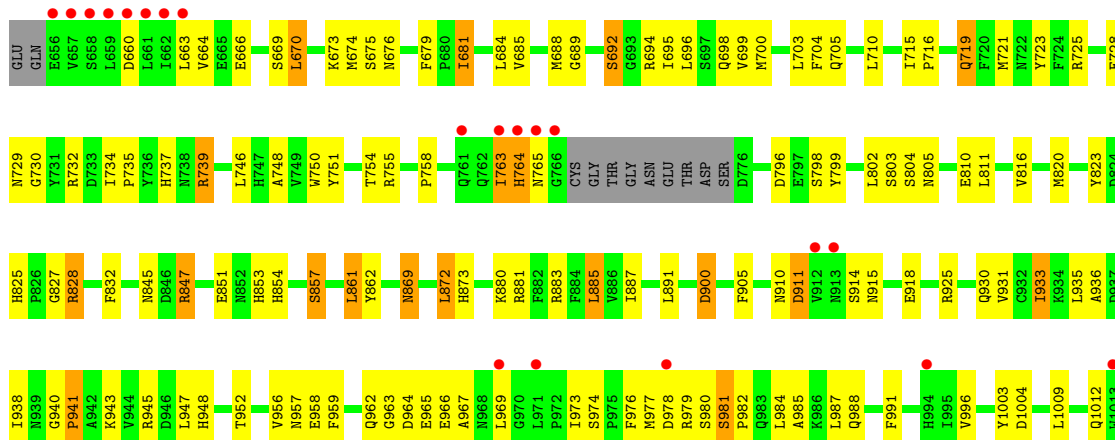
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

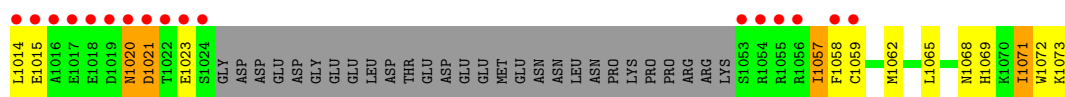
Chain K:



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

Chain L:





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 275.05Å 147.08Å 253.49Å 90.00° 109.84° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.90 49.61 – 2.90 | Depositor EDS |
| % Data completeness (in resolution range) | 97.7 (30.00-2.90) 96.6 (49.61-2.90) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.14 (at 2.91Å) | Xtriage |
| Refinement program | CNX | Depositor |
| R, R_{free} | 0.231 , 0.249 0.228 , 0.242 | Depositor DCC |
| R_{free} test set | 10128 reflections (5.24%) | DCC |
| Wilson B-factor (Å ²) | 49.3 | Xtriage |
| Anisotropy | 0.691 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 24.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 0 of 203261 reflections | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 36048 | wwPDB-VP |
| Average B, all atoms (Å ²) | 48.0 | 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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.45 | 0/2982 | 0.59 | 0/4053 |
| 1 | B | 0.44 | 0/3092 | 0.59 | 0/4203 |
| 1 | C | 0.45 | 0/2982 | 0.59 | 0/4053 |
| 1 | D | 0.47 | 0/3092 | 0.60 | 0/4203 |
| 1 | E | 0.47 | 1/2982 (0.0%) | 0.59 | 0/4053 |
| 1 | F | 0.46 | 0/3092 | 0.59 | 0/4203 |
| 1 | G | 0.45 | 0/2982 | 0.59 | 0/4053 |
| 1 | H | 0.45 | 0/3092 | 0.59 | 1/4203 (0.0%) |
| 1 | I | 0.45 | 0/2982 | 0.58 | 0/4053 |
| 1 | J | 0.46 | 0/3092 | 0.59 | 0/4203 |
| 1 | K | 0.47 | 0/2982 | 0.59 | 0/4053 |
| 1 | L | 0.47 | 0/3092 | 0.60 | 0/4203 |
| All | All | 0.46 | 1/36444 (0.0%) | 0.59 | 1/49536 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | E | 1000 | CYS | CB-SG | -5.15 | 1.73 | 1.81 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | H | 795 | PRO | N-CA-CB | 5.03 | 109.34 | 103.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2907 | 0 | 2772 | 110 | 0 |
| 1 | B | 3017 | 0 | 2834 | 132 | 0 |
| 1 | C | 2907 | 0 | 2772 | 124 | 0 |
| 1 | D | 3017 | 0 | 2834 | 134 | 0 |
| 1 | E | 2907 | 0 | 2772 | 114 | 0 |
| 1 | F | 3017 | 0 | 2834 | 119 | 0 |
| 1 | G | 2907 | 0 | 2772 | 109 | 0 |
| 1 | H | 3017 | 0 | 2834 | 126 | 0 |
| 1 | I | 2907 | 0 | 2772 | 108 | 0 |
| 1 | J | 3017 | 0 | 2834 | 143 | 0 |
| 1 | K | 2907 | 0 | 2772 | 108 | 0 |
| 1 | L | 3017 | 0 | 2834 | 125 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 2 | C | 2 | 0 | 0 | 0 | 0 |
| 2 | D | 2 | 0 | 0 | 0 | 0 |
| 2 | E | 2 | 0 | 0 | 0 | 0 |
| 2 | F | 2 | 0 | 0 | 0 | 0 |
| 2 | G | 2 | 0 | 0 | 0 | 0 |
| 2 | H | 2 | 0 | 0 | 0 | 0 |
| 2 | I | 2 | 0 | 0 | 0 | 0 |
| 2 | J | 2 | 0 | 0 | 0 | 0 |
| 2 | K | 2 | 0 | 0 | 0 | 0 |
| 2 | L | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 16 | 0 | 14 | 0 | 0 |
| 3 | B | 16 | 0 | 14 | 0 | 0 |
| 3 | C | 16 | 0 | 14 | 0 | 0 |
| 3 | D | 16 | 0 | 14 | 0 | 0 |
| 3 | E | 16 | 0 | 14 | 0 | 0 |
| 3 | F | 16 | 0 | 14 | 0 | 0 |
| 3 | G | 16 | 0 | 14 | 0 | 0 |
| 3 | H | 16 | 0 | 14 | 0 | 0 |
| 3 | I | 16 | 0 | 14 | 0 | 0 |
| 3 | J | 16 | 0 | 14 | 0 | 0 |
| 3 | K | 16 | 0 | 14 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | L | 16 | 0 | 14 | 0 | 0 |
| 4 | A | 24 | 0 | 0 | 1 | 0 |
| 4 | B | 24 | 0 | 0 | 3 | 0 |
| 4 | C | 24 | 0 | 0 | 1 | 0 |
| 4 | D | 24 | 0 | 0 | 1 | 0 |
| 4 | E | 23 | 0 | 0 | 2 | 0 |
| 4 | F | 25 | 0 | 0 | 1 | 0 |
| 4 | G | 23 | 0 | 0 | 1 | 0 |
| 4 | H | 25 | 0 | 0 | 0 | 0 |
| 4 | I | 24 | 0 | 0 | 1 | 0 |
| 4 | J | 24 | 0 | 0 | 0 | 0 |
| 4 | K | 24 | 0 | 0 | 1 | 0 |
| 4 | L | 24 | 0 | 0 | 1 | 0 |
| All | All | 36048 | 0 | 33804 | 1360 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (1360) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:E:825:HIS:HD2 | 1:E:827:GLY:H | 1.10 | 1.00 |
| 1:A:719:GLN:H | 1:A:719:GLN:HE21 | 1.04 | 1.00 |
| 1:I:719:GLN:HE21 | 1:I:719:GLN:H | 1.06 | 0.98 |
| 1:K:762:GLN:HE22 | 1:K:804:SER:HB2 | 1.28 | 0.98 |
| 1:K:719:GLN:H | 1:K:719:GLN:HE21 | 1.06 | 0.98 |
| 1:E:719:GLN:H | 1:E:719:GLN:HE21 | 1.05 | 0.97 |
| 1:G:719:GLN:HE21 | 1:G:719:GLN:H | 1.05 | 0.96 |
| 1:G:1014:LEU:HD12 | 1:G:1056:ARG:HB3 | 1.45 | 0.96 |
| 1:I:825:HIS:HD2 | 1:I:827:GLY:H | 1.09 | 0.96 |
| 1:L:719:GLN:HE21 | 1:L:719:GLN:N | 1.64 | 0.95 |
| 1:C:825:HIS:HD2 | 1:C:827:GLY:H | 1.10 | 0.95 |
| 1:B:719:GLN:HE21 | 1:B:719:GLN:N | 1.63 | 0.95 |
| 1:C:719:GLN:HE21 | 1:C:719:GLN:H | 1.10 | 0.95 |
| 1:F:719:GLN:N | 1:F:719:GLN:HE21 | 1.63 | 0.94 |
| 1:D:719:GLN:HE21 | 1:D:719:GLN:N | 1.65 | 0.94 |
| 1:H:719:GLN:HE21 | 1:H:719:GLN:N | 1.64 | 0.94 |
| 1:G:825:HIS:HD2 | 1:G:827:GLY:H | 1.11 | 0.94 |
| 1:J:719:GLN:N | 1:J:719:GLN:HE21 | 1.64 | 0.94 |
| 1:B:719:GLN:NE2 | 1:B:719:GLN:H | 1.64 | 0.94 |
| 1:F:719:GLN:H | 1:F:719:GLN:NE2 | 1.65 | 0.94 |
| 1:A:825:HIS:HD2 | 1:A:827:GLY:H | 1.09 | 0.94 |
| 1:L:719:GLN:NE2 | 1:L:719:GLN:H | 1.66 | 0.93 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:L:911:ASP:H | 1:L:914:SER:HB3 | 1.34 | 0.93 |
| 1:H:719:GLN:NE2 | 1:H:719:GLN:H | 1.66 | 0.93 |
| 1:J:719:GLN:H | 1:J:719:GLN:NE2 | 1.65 | 0.93 |
| 1:B:911:ASP:H | 1:B:914:SER:HB3 | 1.33 | 0.92 |
| 1:D:719:GLN:NE2 | 1:D:719:GLN:H | 1.67 | 0.92 |
| 1:F:911:ASP:H | 1:F:914:SER:HB3 | 1.33 | 0.92 |
| 1:K:825:HIS:HD2 | 1:K:827:GLY:H | 1.10 | 0.91 |
| 1:D:911:ASP:H | 1:D:914:SER:HB3 | 1.36 | 0.90 |
| 1:A:762:GLN:HE21 | 1:A:801:CYS:H | 1.19 | 0.90 |
| 1:H:911:ASP:H | 1:H:914:SER:HB3 | 1.34 | 0.89 |
| 1:J:911:ASP:H | 1:J:914:SER:HB3 | 1.34 | 0.89 |
| 1:H:828:ARG:HG2 | 1:H:832:PHE:CD2 | 2.08 | 0.89 |
| 1:K:762:GLN:HA | 1:K:762:GLN:HE21 | 1.37 | 0.88 |
| 1:F:828:ARG:HG2 | 1:F:832:PHE:CD2 | 2.08 | 0.88 |
| 1:K:730:GLY:HA3 | 1:K:823:TYR:CE1 | 2.08 | 0.88 |
| 1:A:730:GLY:HA3 | 1:A:823:TYR:CE1 | 2.09 | 0.87 |
| 1:J:828:ARG:HG2 | 1:J:832:PHE:CD2 | 2.09 | 0.87 |
| 1:B:828:ARG:HG2 | 1:B:832:PHE:CD2 | 2.09 | 0.86 |
| 1:E:730:GLY:HA3 | 1:E:823:TYR:CE1 | 2.11 | 0.86 |
| 1:I:754:THR:HG21 | 1:I:755:ARG:HH21 | 1.38 | 0.86 |
| 1:G:730:GLY:HA3 | 1:G:823:TYR:CE1 | 2.11 | 0.86 |
| 1:F:758:PRO:HG2 | 1:F:1057:ILE:HD13 | 1.56 | 0.86 |
| 1:D:828:ARG:HG2 | 1:D:832:PHE:CD2 | 2.10 | 0.86 |
| 1:L:828:ARG:HG2 | 1:L:832:PHE:CD2 | 2.11 | 0.85 |
| 1:G:754:THR:HG21 | 1:G:755:ARG:HH21 | 1.39 | 0.85 |
| 1:C:754:THR:HG21 | 1:C:755:ARG:HH21 | 1.39 | 0.85 |
| 1:J:758:PRO:HG2 | 1:J:1057:ILE:HD13 | 1.59 | 0.85 |
| 1:A:754:THR:HG21 | 1:A:755:ARG:HH21 | 1.41 | 0.84 |
| 1:A:719:GLN:N | 1:A:719:GLN:HE21 | 1.74 | 0.84 |
| 1:C:730:GLY:HA3 | 1:C:823:TYR:CE1 | 2.11 | 0.84 |
| 1:D:825:HIS:HD2 | 1:D:827:GLY:H | 1.25 | 0.84 |
| 1:I:730:GLY:HA3 | 1:I:823:TYR:CE1 | 2.11 | 0.84 |
| 1:K:754:THR:HG21 | 1:K:755:ARG:HH21 | 1.39 | 0.84 |
| 1:G:719:GLN:N | 1:G:719:GLN:HE21 | 1.75 | 0.83 |
| 1:C:754:THR:HG22 | 1:C:755:ARG:HE | 1.44 | 0.83 |
| 1:H:825:HIS:HD2 | 1:H:827:GLY:H | 1.25 | 0.83 |
| 1:E:719:GLN:N | 1:E:719:GLN:HE21 | 1.75 | 0.83 |
| 1:I:754:THR:HG22 | 1:I:755:ARG:HE | 1.43 | 0.83 |
| 1:E:754:THR:HG21 | 1:E:755:ARG:HH21 | 1.41 | 0.83 |
| 1:I:719:GLN:HE21 | 1:I:719:GLN:N | 1.76 | 0.83 |
| 1:F:825:HIS:HD2 | 1:F:827:GLY:H | 1.25 | 0.82 |
| 1:K:719:GLN:HE21 | 1:K:719:GLN:N | 1.75 | 0.82 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1014:LEU:HD12 | 1:B:1056:ARG:HB3 | 1.61 | 0.82 |
| 1:A:754:THR:HG22 | 1:A:755:ARG:HE | 1.44 | 0.82 |
| 1:L:825:HIS:HD2 | 1:L:827:GLY:H | 1.25 | 0.82 |
| 1:G:754:THR:HG22 | 1:G:755:ARG:HE | 1.45 | 0.81 |
| 1:C:828:ARG:HG2 | 1:C:832:PHE:CD2 | 2.16 | 0.81 |
| 1:A:705:GLN:HE22 | 1:J:1056:ARG:HH21 | 1.25 | 0.81 |
| 1:G:828:ARG:HG2 | 1:G:832:PHE:CD2 | 2.16 | 0.81 |
| 1:C:887:ILE:HD13 | 1:D:845:ASN:HB3 | 1.63 | 0.80 |
| 1:J:825:HIS:HD2 | 1:J:827:GLY:H | 1.24 | 0.80 |
| 1:A:762:GLN:HE21 | 1:A:801:CYS:N | 1.79 | 0.80 |
| 1:A:887:ILE:HD13 | 1:B:845:ASN:HB3 | 1.63 | 0.80 |
| 1:C:719:GLN:N | 1:C:719:GLN:HE21 | 1.79 | 0.80 |
| 1:K:754:THR:HG22 | 1:K:755:ARG:HE | 1.44 | 0.80 |
| 1:B:825:HIS:HD2 | 1:B:827:GLY:H | 1.26 | 0.80 |
| 1:E:828:ARG:HG2 | 1:E:832:PHE:CD2 | 2.17 | 0.79 |
| 1:C:959:PHE:HB3 | 1:C:977:MET:HG2 | 1.64 | 0.79 |
| 1:L:739:ARG:HG2 | 1:L:739:ARG:HH11 | 1.48 | 0.79 |
| 1:E:754:THR:HG22 | 1:E:755:ARG:HE | 1.47 | 0.79 |
| 1:I:737:HIS:HD2 | 1:I:958:GLU:OE2 | 1.66 | 0.78 |
| 1:A:828:ARG:HG2 | 1:A:832:PHE:CD2 | 2.18 | 0.78 |
| 1:G:719:GLN:NE2 | 1:G:719:GLN:H | 1.82 | 0.77 |
| 1:A:959:PHE:HB3 | 1:A:977:MET:HG2 | 1.65 | 0.77 |
| 1:D:739:ARG:HG2 | 1:D:739:ARG:HH11 | 1.50 | 0.77 |
| 1:E:737:HIS:HD2 | 1:E:958:GLU:OE2 | 1.67 | 0.77 |
| 1:K:762:GLN:NE2 | 1:K:804:SER:HB2 | 1.98 | 0.77 |
| 1:K:828:ARG:HG2 | 1:K:832:PHE:CD2 | 2.20 | 0.77 |
| 1:I:883:ARG:NH1 | 1:J:846:ASP:OD2 | 2.18 | 0.77 |
| 1:G:959:PHE:HB3 | 1:G:977:MET:HG2 | 1.65 | 0.77 |
| 1:D:758:PRO:HG2 | 1:D:1057:ILE:HD13 | 1.66 | 0.77 |
| 1:G:913:ASN:ND2 | 1:K:1056:ARG:HH21 | 1.83 | 0.76 |
| 1:A:737:HIS:HD2 | 1:A:958:GLU:OE2 | 1.66 | 0.76 |
| 1:J:739:ARG:HH11 | 1:J:739:ARG:HG2 | 1.48 | 0.76 |
| 1:B:739:ARG:HG2 | 1:B:739:ARG:HH11 | 1.50 | 0.76 |
| 1:L:730:GLY:HA3 | 1:L:823:TYR:CE1 | 2.20 | 0.76 |
| 1:F:730:GLY:HA3 | 1:F:823:TYR:CE1 | 2.21 | 0.76 |
| 1:K:887:ILE:HD13 | 1:L:845:ASN:HB3 | 1.64 | 0.76 |
| 1:E:719:GLN:H | 1:E:719:GLN:NE2 | 1.83 | 0.76 |
| 1:E:959:PHE:HB3 | 1:E:977:MET:HG2 | 1.67 | 0.76 |
| 1:C:737:HIS:HD2 | 1:C:958:GLU:OE2 | 1.67 | 0.75 |
| 1:J:730:GLY:HA3 | 1:J:823:TYR:CE1 | 2.21 | 0.75 |
| 1:I:828:ARG:HG2 | 1:I:832:PHE:CD2 | 2.19 | 0.75 |
| 1:D:754:THR:HG21 | 1:D:755:ARG:HH21 | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:K:737:HIS:HD2 | 1:K:958:GLU:OE2 | 1.68 | 0.75 |
| 1:H:739:ARG:HG2 | 1:H:739:ARG:HH11 | 1.51 | 0.75 |
| 1:K:696:LEU:HB3 | 1:K:728:GLU:HG2 | 1.68 | 0.75 |
| 1:K:719:GLN:H | 1:K:719:GLN:NE2 | 1.83 | 0.74 |
| 1:E:1014:LEU:HD12 | 1:E:1056:ARG:HB3 | 1.69 | 0.74 |
| 1:D:730:GLY:HA3 | 1:D:823:TYR:CE1 | 2.22 | 0.74 |
| 1:J:754:THR:HG21 | 1:J:755:ARG:HH21 | 1.52 | 0.74 |
| 1:I:696:LEU:HB3 | 1:I:728:GLU:HG2 | 1.70 | 0.74 |
| 1:H:754:THR:HG21 | 1:H:755:ARG:HH21 | 1.53 | 0.74 |
| 1:H:730:GLY:HA3 | 1:H:823:TYR:CE1 | 2.22 | 0.74 |
| 1:F:700:MET:HE2 | 1:F:746:LEU:HD21 | 1.70 | 0.73 |
| 1:I:959:PHE:HB3 | 1:I:977:MET:HG2 | 1.69 | 0.73 |
| 1:G:1014:LEU:HD12 | 1:G:1056:ARG:CB | 2.18 | 0.73 |
| 1:F:739:ARG:HH11 | 1:F:739:ARG:HG2 | 1.51 | 0.73 |
| 1:F:911:ASP:N | 1:F:914:SER:HB3 | 2.03 | 0.73 |
| 1:B:1057:ILE:HD12 | 1:B:1058:PHE:N | 2.03 | 0.73 |
| 1:A:705:GLN:NE2 | 1:J:1056:ARG:HH21 | 1.87 | 0.73 |
| 1:F:754:THR:HG21 | 1:F:755:ARG:HH21 | 1.52 | 0.73 |
| 1:E:887:ILE:HD13 | 1:F:845:ASN:HB3 | 1.71 | 0.73 |
| 1:C:696:LEU:HB3 | 1:C:728:GLU:HG2 | 1.70 | 0.72 |
| 1:B:754:THR:HG21 | 1:B:755:ARG:HH21 | 1.54 | 0.72 |
| 1:A:719:GLN:H | 1:A:719:GLN:NE2 | 1.82 | 0.72 |
| 1:L:911:ASP:N | 1:L:914:SER:HB3 | 2.04 | 0.72 |
| 1:B:911:ASP:N | 1:B:914:SER:HB3 | 2.02 | 0.72 |
| 1:B:730:GLY:HA3 | 1:B:823:TYR:CE1 | 2.24 | 0.72 |
| 1:H:696:LEU:HB3 | 1:H:728:GLU:HG2 | 1.70 | 0.72 |
| 1:F:1057:ILE:HD12 | 1:F:1058:PHE:N | 2.03 | 0.72 |
| 1:K:959:PHE:HB3 | 1:K:977:MET:HG2 | 1.70 | 0.72 |
| 1:J:911:ASP:N | 1:J:914:SER:HB3 | 2.03 | 0.72 |
| 1:A:696:LEU:HB3 | 1:A:728:GLU:HG2 | 1.71 | 0.72 |
| 1:G:1017:GLU:HB3 | 1:G:1055:ARG:HD3 | 1.72 | 0.72 |
| 1:G:737:HIS:HD2 | 1:G:958:GLU:OE2 | 1.71 | 0.72 |
| 1:E:696:LEU:HB3 | 1:E:728:GLU:HG2 | 1.71 | 0.72 |
| 1:F:696:LEU:HB3 | 1:F:728:GLU:HG2 | 1.71 | 0.72 |
| 1:F:1059:CYS:HB3 | 1:F:1062:MET:HB2 | 1.72 | 0.71 |
| 1:D:911:ASP:N | 1:D:914:SER:HB3 | 2.05 | 0.71 |
| 1:L:696:LEU:HB3 | 1:L:728:GLU:HG2 | 1.70 | 0.71 |
| 1:J:1057:ILE:HD12 | 1:J:1058:PHE:N | 2.06 | 0.71 |
| 1:G:696:LEU:HB3 | 1:G:728:GLU:HG2 | 1.72 | 0.71 |
| 1:H:956:VAL:HG11 | 1:H:984:LEU:HD13 | 1.72 | 0.71 |
| 1:B:696:LEU:HB3 | 1:B:728:GLU:HG2 | 1.71 | 0.71 |
| 1:C:1017:GLU:H | 1:C:1055:ARG:HD3 | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:L:956:VAL:HG11 | 1:L:984:LEU:HD13 | 1.72 | 0.71 |
| 1:E:1017:GLU:HB3 | 1:E:1055:ARG:HD3 | 1.73 | 0.70 |
| 1:D:956:VAL:HG11 | 1:D:984:LEU:HD13 | 1.72 | 0.70 |
| 1:B:915:ASN:CG | 1:C:945:ARG:NH1 | 2.45 | 0.70 |
| 1:B:956:VAL:HG11 | 1:B:984:LEU:HD13 | 1.73 | 0.70 |
| 1:L:754:THR:HG21 | 1:L:755:ARG:HH21 | 1.56 | 0.70 |
| 1:H:1013:TRP:CE3 | 1:H:1057:ILE:HG22 | 2.27 | 0.70 |
| 1:I:891:LEU:HD13 | 1:J:847:ARG:NH2 | 2.06 | 0.70 |
| 1:H:911:ASP:N | 1:H:914:SER:HB3 | 2.04 | 0.69 |
| 1:I:719:GLN:NE2 | 1:I:719:GLN:H | 1.84 | 0.69 |
| 1:H:945:ARG:HH12 | 1:H:1071:ILE:HG21 | 1.57 | 0.69 |
| 1:F:956:VAL:HG11 | 1:F:984:LEU:HD13 | 1.73 | 0.69 |
| 1:J:696:LEU:HB3 | 1:J:728:GLU:HG2 | 1.73 | 0.69 |
| 1:J:956:VAL:HG11 | 1:J:984:LEU:HD13 | 1.73 | 0.69 |
| 1:D:696:LEU:HB3 | 1:D:728:GLU:HG2 | 1.73 | 0.69 |
| 1:I:762:GLN:NE2 | 1:I:801:CYS:H | 1.91 | 0.68 |
| 1:C:719:GLN:NE2 | 1:C:719:GLN:H | 1.87 | 0.68 |
| 1:L:853:HIS:O | 1:L:857:SER:HB2 | 1.94 | 0.68 |
| 1:F:853:HIS:O | 1:F:857:SER:HB2 | 1.93 | 0.68 |
| 1:F:945:ARG:HH12 | 1:F:1071:ILE:HG21 | 1.59 | 0.68 |
| 1:H:1056:ARG:HH11 | 1:H:1056:ARG:HB3 | 1.58 | 0.67 |
| 1:H:853:HIS:O | 1:H:857:SER:HB2 | 1.94 | 0.67 |
| 1:H:816:VAL:O | 1:H:820:MET:HG2 | 1.95 | 0.67 |
| 1:I:891:LEU:CD1 | 1:J:847:ARG:CZ | 2.73 | 0.67 |
| 1:B:853:HIS:O | 1:B:857:SER:HB2 | 1.94 | 0.67 |
| 1:D:853:HIS:O | 1:D:857:SER:HB2 | 1.94 | 0.67 |
| 1:C:845:ASN:HB3 | 1:D:887:ILE:HD13 | 1.77 | 0.66 |
| 1:H:689:GLY:O | 1:H:692:SER:HB3 | 1.95 | 0.66 |
| 1:B:915:ASN:ND2 | 1:C:945:ARG:HH11 | 1.92 | 0.66 |
| 1:D:816:VAL:O | 1:D:820:MET:HG2 | 1.96 | 0.66 |
| 1:D:945:ARG:HH12 | 1:D:1071:ILE:HG21 | 1.60 | 0.66 |
| 1:L:734:ILE:HB | 1:L:735:PRO:HD2 | 1.77 | 0.66 |
| 1:F:816:VAL:O | 1:F:820:MET:HG2 | 1.96 | 0.66 |
| 1:B:689:GLY:O | 1:B:692:SER:HB3 | 1.95 | 0.66 |
| 1:J:853:HIS:O | 1:J:857:SER:HB2 | 1.96 | 0.66 |
| 1:J:945:ARG:HH12 | 1:J:1071:ILE:HG21 | 1.59 | 0.66 |
| 1:B:761:GLN:HG2 | 1:B:763:ILE:H | 1.60 | 0.66 |
| 1:L:816:VAL:O | 1:L:820:MET:HG2 | 1.96 | 0.65 |
| 1:G:739:ARG:HG2 | 4:G:1423:HOH:O | 1.95 | 0.65 |
| 1:A:825:HIS:CD2 | 1:A:827:GLY:H | 2.02 | 0.65 |
| 1:J:734:ILE:HB | 1:J:735:PRO:HD2 | 1.77 | 0.65 |
| 1:L:734:ILE:HD11 | 1:L:737:HIS:HB2 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:979:ARG:O | 1:B:982:PRO:HD3 | 1.96 | 0.65 |
| 1:L:700:MET:HE2 | 1:L:746:LEU:HD21 | 1.78 | 0.65 |
| 1:L:945:ARG:HH12 | 1:L:1071:ILE:HG21 | 1.60 | 0.65 |
| 1:F:734:ILE:HB | 1:F:735:PRO:HD2 | 1.78 | 0.65 |
| 1:C:700:MET:HE3 | 1:C:746:LEU:HD21 | 1.78 | 0.65 |
| 1:A:700:MET:HE3 | 1:A:746:LEU:HD21 | 1.79 | 0.65 |
| 1:D:734:ILE:HD11 | 1:D:737:HIS:HB2 | 1.78 | 0.65 |
| 1:G:887:ILE:HD13 | 1:H:845:ASN:HB3 | 1.78 | 0.65 |
| 1:K:700:MET:HE3 | 1:K:746:LEU:HD21 | 1.79 | 0.65 |
| 1:H:734:ILE:HD11 | 1:H:737:HIS:HB2 | 1.79 | 0.65 |
| 1:B:734:ILE:HD11 | 1:B:737:HIS:HB2 | 1.79 | 0.65 |
| 1:D:689:GLY:O | 1:D:692:SER:HB3 | 1.97 | 0.65 |
| 1:I:825:HIS:CD2 | 1:I:827:GLY:H | 2.01 | 0.64 |
| 1:B:700:MET:HE2 | 1:B:746:LEU:HD21 | 1.77 | 0.64 |
| 1:B:945:ARG:HH12 | 1:B:1071:ILE:HG21 | 1.61 | 0.64 |
| 1:B:816:VAL:O | 1:B:820:MET:HG2 | 1.97 | 0.64 |
| 1:A:845:ASN:HB3 | 1:B:887:ILE:HD13 | 1.79 | 0.64 |
| 1:E:700:MET:HE3 | 1:E:746:LEU:HD21 | 1.80 | 0.64 |
| 1:D:754:THR:HG22 | 1:D:755:ARG:HE | 1.62 | 0.64 |
| 1:E:1017:GLU:H | 1:E:1055:ARG:HD3 | 1.62 | 0.64 |
| 1:F:689:GLY:O | 1:F:692:SER:HB3 | 1.97 | 0.64 |
| 1:J:739:ARG:NH1 | 1:J:739:ARG:HG2 | 2.11 | 0.64 |
| 1:E:1014:LEU:HD12 | 1:E:1056:ARG:CB | 2.27 | 0.64 |
| 1:H:979:ARG:O | 1:H:982:PRO:HD3 | 1.96 | 0.64 |
| 1:H:739:ARG:HG2 | 1:H:739:ARG:NH1 | 2.13 | 0.64 |
| 1:I:887:ILE:HD13 | 1:J:845:ASN:HB3 | 1.80 | 0.64 |
| 1:F:734:ILE:HD11 | 1:F:737:HIS:HB2 | 1.80 | 0.63 |
| 1:B:734:ILE:HB | 1:B:735:PRO:HD2 | 1.79 | 0.63 |
| 1:A:739:ARG:HG2 | 4:A:1123:HOH:O | 1.98 | 0.63 |
| 1:L:739:ARG:HG2 | 1:L:739:ARG:NH1 | 2.10 | 0.63 |
| 1:K:825:HIS:CD2 | 1:K:827:GLY:H | 2.03 | 0.63 |
| 1:J:1013:TRP:CZ3 | 1:J:1055:ARG:HB3 | 2.33 | 0.63 |
| 1:G:700:MET:HE3 | 1:G:746:LEU:HD21 | 1.79 | 0.63 |
| 1:J:816:VAL:O | 1:J:820:MET:HG2 | 1.99 | 0.63 |
| 1:I:762:GLN:HA | 1:I:805:ASN:HD21 | 1.62 | 0.63 |
| 1:J:689:GLY:O | 1:J:692:SER:HB3 | 1.98 | 0.63 |
| 1:L:689:GLY:O | 1:L:692:SER:HB3 | 1.98 | 0.63 |
| 1:I:707:THR:HG23 | 1:I:787:ILE:HD12 | 1.81 | 0.63 |
| 1:B:739:ARG:HG2 | 1:B:739:ARG:NH1 | 2.12 | 0.63 |
| 1:F:739:ARG:NH1 | 1:F:739:ARG:HG2 | 2.14 | 0.63 |
| 1:E:902:LEU:HD11 | 1:E:999:LEU:HA | 1.81 | 0.63 |
| 1:L:979:ARG:O | 1:L:982:PRO:HD3 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:902:LEU:HD11 | 1:A:999:LEU:HA | 1.80 | 0.63 |
| 1:L:758:PRO:HG2 | 1:L:1057:ILE:HG13 | 1.80 | 0.63 |
| 1:E:707:THR:HG23 | 1:E:787:ILE:HD12 | 1.81 | 0.62 |
| 1:I:700:MET:HE3 | 1:I:746:LEU:HD21 | 1.80 | 0.62 |
| 1:A:762:GLN:HA | 1:A:805:ASN:HD21 | 1.63 | 0.62 |
| 1:J:734:ILE:HD11 | 1:J:737:HIS:HB2 | 1.82 | 0.62 |
| 1:L:825:HIS:CD2 | 1:L:827:GLY:H | 2.14 | 0.62 |
| 1:A:945:ARG:HD3 | 1:D:915:ASN:HD21 | 1.63 | 0.62 |
| 1:I:902:LEU:HD11 | 1:I:999:LEU:HA | 1.81 | 0.62 |
| 1:K:902:LEU:HD11 | 1:K:999:LEU:HA | 1.81 | 0.62 |
| 1:B:934:LYS:HD3 | 4:B:1135:HOH:O | 1.99 | 0.62 |
| 1:C:1056:ARG:HH11 | 1:C:1056:ARG:HG3 | 1.64 | 0.62 |
| 1:K:911:ASP:HB3 | 1:K:914:SER:HB3 | 1.82 | 0.62 |
| 1:G:700:MET:HE3 | 1:G:746:LEU:CD2 | 2.30 | 0.62 |
| 1:L:692:SER:O | 1:L:695:ILE:HG13 | 2.00 | 0.62 |
| 1:C:911:ASP:HB3 | 1:C:914:SER:HB3 | 1.82 | 0.62 |
| 1:B:825:HIS:CD2 | 1:B:827:GLY:H | 2.15 | 0.61 |
| 1:G:913:ASN:HD22 | 1:K:1056:ARG:HH21 | 1.47 | 0.61 |
| 1:C:718:GLN:HG3 | 1:C:722:ASN:HD21 | 1.65 | 0.61 |
| 1:G:902:LEU:HD11 | 1:G:999:LEU:HA | 1.82 | 0.61 |
| 1:C:707:THR:HG23 | 1:C:787:ILE:HD12 | 1.80 | 0.61 |
| 1:I:825:HIS:HD2 | 1:I:827:GLY:N | 1.91 | 0.61 |
| 1:K:700:MET:HE3 | 1:K:746:LEU:CD2 | 2.31 | 0.61 |
| 1:H:734:ILE:HB | 1:H:735:PRO:HD2 | 1.80 | 0.61 |
| 1:C:902:LEU:HD11 | 1:C:999:LEU:HA | 1.83 | 0.61 |
| 1:A:917:ILE:O | 1:A:918:GLU:HB2 | 2.01 | 0.61 |
| 1:I:700:MET:HE3 | 1:I:746:LEU:CD2 | 2.30 | 0.61 |
| 1:L:719:GLN:HE21 | 1:L:719:GLN:H | 0.81 | 0.61 |
| 1:G:707:THR:HG23 | 1:G:787:ILE:HD12 | 1.83 | 0.61 |
| 1:C:825:HIS:CD2 | 1:C:827:GLY:H | 2.03 | 0.61 |
| 1:H:692:SER:O | 1:H:695:ILE:HG13 | 2.00 | 0.61 |
| 1:C:700:MET:HE3 | 1:C:746:LEU:CD2 | 2.31 | 0.61 |
| 1:A:945:ARG:CD | 1:D:915:ASN:HD21 | 2.13 | 0.61 |
| 1:K:707:THR:HG23 | 1:K:787:ILE:HD12 | 1.83 | 0.61 |
| 1:J:1058:PHE:CE1 | 1:J:1063:HIS:CE1 | 2.88 | 0.60 |
| 1:J:692:SER:O | 1:J:695:ILE:HG13 | 2.01 | 0.60 |
| 1:E:825:HIS:CD2 | 1:E:827:GLY:H | 2.03 | 0.60 |
| 1:J:1057:ILE:HD12 | 1:J:1058:PHE:H | 1.65 | 0.60 |
| 1:J:825:HIS:CD2 | 1:J:827:GLY:H | 2.13 | 0.60 |
| 1:I:891:LEU:HD12 | 1:J:847:ARG:NH1 | 2.16 | 0.60 |
| 1:A:707:THR:HG23 | 1:A:787:ILE:HD12 | 1.82 | 0.60 |
| 1:A:911:ASP:HB3 | 1:A:914:SER:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:700:MET:HE2 | 1:J:746:LEU:HD21 | 1.82 | 0.60 |
| 1:E:845:ASN:HB3 | 1:F:887:ILE:HD13 | 1.82 | 0.60 |
| 1:A:945:ARG:HH11 | 1:D:915:ASN:ND2 | 1.99 | 0.60 |
| 1:A:825:HIS:HD2 | 1:A:827:GLY:N | 1.92 | 0.60 |
| 1:J:754:THR:HG22 | 1:J:755:ARG:HE | 1.67 | 0.60 |
| 1:F:692:SER:O | 1:F:695:ILE:HG13 | 2.02 | 0.60 |
| 1:D:700:MET:HE2 | 1:D:746:LEU:HD21 | 1.83 | 0.60 |
| 1:J:725:ARG:HH11 | 1:J:725:ARG:HG3 | 1.67 | 0.60 |
| 1:K:719:GLN:HA | 1:K:722:ASN:HD22 | 1.67 | 0.60 |
| 1:J:1003:TYR:CD2 | 1:J:1009:LEU:HG | 2.36 | 0.60 |
| 1:I:911:ASP:HB3 | 1:I:914:SER:HB3 | 1.83 | 0.60 |
| 1:K:679:PHE:HZ | 1:K:684:LEU:HD12 | 1.67 | 0.60 |
| 1:I:891:LEU:HD12 | 1:J:847:ARG:CZ | 2.32 | 0.60 |
| 1:D:734:ILE:HB | 1:D:735:PRO:HD2 | 1.82 | 0.60 |
| 1:G:911:ASP:HB3 | 1:G:914:SER:HB3 | 1.82 | 0.60 |
| 1:I:845:ASN:HB3 | 1:J:887:ILE:HD13 | 1.83 | 0.59 |
| 1:A:945:ARG:NH1 | 1:D:915:ASN:CG | 2.55 | 0.59 |
| 1:E:911:ASP:HB3 | 1:E:914:SER:HB3 | 1.84 | 0.59 |
| 1:F:754:THR:HG22 | 1:F:755:ARG:HE | 1.67 | 0.59 |
| 1:D:692:SER:O | 1:D:695:ILE:HG13 | 2.02 | 0.59 |
| 1:A:707:THR:CG2 | 1:A:709:LEU:HG | 2.33 | 0.59 |
| 1:E:718:GLN:HG3 | 1:E:722:ASN:HD21 | 1.67 | 0.59 |
| 1:H:754:THR:HG22 | 1:H:755:ARG:HE | 1.67 | 0.59 |
| 1:G:825:HIS:CD2 | 1:G:827:GLY:H | 2.04 | 0.59 |
| 1:B:692:SER:O | 1:B:695:ILE:HG13 | 2.02 | 0.59 |
| 1:E:700:MET:HE3 | 1:E:746:LEU:CD2 | 2.33 | 0.59 |
| 1:F:1003:TYR:CD2 | 1:F:1009:LEU:HG | 2.38 | 0.59 |
| 1:L:754:THR:HG22 | 1:L:755:ARG:HE | 1.68 | 0.59 |
| 1:B:725:ARG:HH11 | 1:B:725:ARG:HG3 | 1.67 | 0.59 |
| 1:H:679:PHE:HZ | 1:H:684:LEU:HD12 | 1.68 | 0.59 |
| 1:L:725:ARG:HH11 | 1:L:725:ARG:HG3 | 1.66 | 0.59 |
| 1:K:707:THR:CG2 | 1:K:709:LEU:HG | 2.32 | 0.58 |
| 1:K:730:GLY:HA3 | 1:K:823:TYR:HE1 | 1.64 | 0.58 |
| 1:H:751:TYR:CZ | 1:H:755:ARG:HG3 | 2.37 | 0.58 |
| 1:F:979:ARG:O | 1:F:982:PRO:HD3 | 2.02 | 0.58 |
| 1:D:739:ARG:HG2 | 1:D:739:ARG:NH1 | 2.13 | 0.58 |
| 1:F:748:ALA:HB3 | 1:F:936:ALA:HB1 | 1.86 | 0.58 |
| 1:C:917:ILE:O | 1:C:918:GLU:HB2 | 2.03 | 0.58 |
| 1:H:825:HIS:CD2 | 1:H:827:GLY:H | 2.14 | 0.58 |
| 1:B:1069:HIS:CE1 | 1:B:1073:LYS:HZ2 | 2.21 | 0.58 |
| 1:G:917:ILE:O | 1:G:918:GLU:HB2 | 2.03 | 0.58 |
| 1:D:979:ARG:O | 1:D:982:PRO:HD3 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C:1017:GLU:HB3 | 1:C:1055:ARG:HD3 | 1.84 | 0.58 |
| 1:A:700:MET:HE3 | 1:A:746:LEU:CD2 | 2.33 | 0.58 |
| 1:C:707:THR:CG2 | 1:C:709:LEU:HG | 2.34 | 0.58 |
| 1:B:941:PRO:O | 1:B:1065:LEU:HD12 | 2.03 | 0.58 |
| 1:I:754:THR:CG2 | 1:I:755:ARG:HH21 | 2.15 | 0.58 |
| 1:L:1003:TYR:CD2 | 1:L:1009:LEU:HG | 2.39 | 0.58 |
| 1:J:1058:PHE:HE1 | 1:J:1063:HIS:ND1 | 2.01 | 0.58 |
| 1:B:754:THR:HG22 | 1:B:755:ARG:HE | 1.69 | 0.58 |
| 1:E:909:ALA:HB2 | 1:E:917:ILE:HD11 | 1.85 | 0.58 |
| 1:J:962:GLN:O | 1:J:966:GLU:HG3 | 2.04 | 0.58 |
| 1:F:669:SER:HB3 | 1:F:673:LYS:NZ | 2.19 | 0.58 |
| 1:E:917:ILE:O | 1:E:918:GLU:HB2 | 2.04 | 0.58 |
| 1:C:883:ARG:NH1 | 1:D:846:ASP:OD2 | 2.36 | 0.58 |
| 1:E:1071:ILE:HG21 | 1:J:915:ASN:ND2 | 2.19 | 0.58 |
| 1:I:883:ARG:HH12 | 1:J:846:ASP:CG | 2.07 | 0.58 |
| 1:B:915:ASN:HD21 | 1:C:945:ARG:CD | 2.16 | 0.58 |
| 1:I:707:THR:CG2 | 1:I:709:LEU:HG | 2.34 | 0.58 |
| 1:H:725:ARG:HG3 | 1:H:725:ARG:HH11 | 1.67 | 0.57 |
| 1:K:909:ALA:HB2 | 1:K:917:ILE:HD11 | 1.85 | 0.57 |
| 1:B:660:ASP:O | 1:B:664:VAL:HG23 | 2.04 | 0.57 |
| 1:F:962:GLN:O | 1:F:966:GLU:HG3 | 2.03 | 0.57 |
| 1:H:669:SER:HB3 | 1:H:673:LYS:NZ | 2.19 | 0.57 |
| 1:K:825:HIS:HD2 | 1:K:827:GLY:N | 1.93 | 0.57 |
| 1:F:1057:ILE:HD12 | 1:F:1058:PHE:H | 1.67 | 0.57 |
| 1:L:748:ALA:HB3 | 1:L:936:ALA:HB1 | 1.86 | 0.57 |
| 1:E:679:PHE:HZ | 1:E:684:LEU:HD12 | 1.69 | 0.57 |
| 1:E:719:GLN:HA | 1:E:722:ASN:HD22 | 1.68 | 0.57 |
| 1:G:718:GLN:HG3 | 1:G:722:ASN:HD21 | 1.69 | 0.57 |
| 1:G:719:GLN:HA | 1:G:722:ASN:HD22 | 1.69 | 0.57 |
| 1:G:909:ALA:HB2 | 1:G:917:ILE:HD11 | 1.85 | 0.57 |
| 1:I:1056:ARG:HG3 | 1:I:1056:ARG:HH11 | 1.69 | 0.57 |
| 1:K:718:GLN:HG3 | 1:K:722:ASN:HD21 | 1.68 | 0.57 |
| 1:E:707:THR:CG2 | 1:E:709:LEU:HG | 2.35 | 0.57 |
| 1:G:1013:TRP:CE3 | 1:G:1057:ILE:HG22 | 2.40 | 0.57 |
| 1:G:679:PHE:HZ | 1:G:684:LEU:HD12 | 1.69 | 0.57 |
| 1:B:1003:TYR:CD2 | 1:B:1009:LEU:HG | 2.40 | 0.57 |
| 1:E:751:TYR:CE2 | 1:E:755:ARG:HG3 | 2.40 | 0.57 |
| 1:L:679:PHE:HZ | 1:L:684:LEU:HD12 | 1.70 | 0.57 |
| 1:F:825:HIS:CD2 | 1:F:827:GLY:H | 2.15 | 0.57 |
| 1:I:718:GLN:HG3 | 1:I:722:ASN:HD21 | 1.69 | 0.57 |
| 1:L:828:ARG:HG2 | 1:L:832:PHE:CG | 2.40 | 0.57 |
| 1:B:751:TYR:CZ | 1:B:755:ARG:HG3 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:H:1003:TYR:CD2 | 1:H:1009:LEU:HG | 2.39 | 0.57 |
| 1:D:725:ARG:HG3 | 1:D:725:ARG:HH11 | 1.69 | 0.57 |
| 1:H:660:ASP:O | 1:H:664:VAL:HG23 | 2.05 | 0.57 |
| 1:I:1013:TRP:CE3 | 1:I:1057:ILE:HG22 | 2.40 | 0.57 |
| 1:I:802:LEU:HD22 | 1:I:802:LEU:H | 1.70 | 0.57 |
| 1:D:952:THR:HG23 | 1:D:988:GLN:NE2 | 2.20 | 0.56 |
| 1:L:1012:GLN:O | 1:L:1057:ILE:HG12 | 2.05 | 0.56 |
| 1:F:725:ARG:HG3 | 1:F:725:ARG:HH11 | 1.70 | 0.56 |
| 1:J:979:ARG:O | 1:J:982:PRO:HD3 | 2.05 | 0.56 |
| 1:H:748:ALA:HB3 | 1:H:936:ALA:HB1 | 1.87 | 0.56 |
| 1:K:845:ASN:HB3 | 1:L:887:ILE:HD13 | 1.86 | 0.56 |
| 1:K:762:GLN:CA | 1:K:762:GLN:HE21 | 2.13 | 0.56 |
| 1:H:719:GLN:HE21 | 1:H:719:GLN:H | 0.81 | 0.56 |
| 1:H:945:ARG:NH1 | 1:H:1071:ILE:HG21 | 2.20 | 0.56 |
| 1:K:917:ILE:O | 1:K:918:GLU:HB2 | 2.04 | 0.56 |
| 1:G:802:LEU:HD22 | 1:G:802:LEU:H | 1.71 | 0.56 |
| 1:D:669:SER:HB3 | 1:D:673:LYS:NZ | 2.20 | 0.56 |
| 1:C:719:GLN:HA | 1:C:722:ASN:HD22 | 1.70 | 0.56 |
| 1:L:669:SER:HB3 | 1:L:673:LYS:NZ | 2.20 | 0.56 |
| 1:D:941:PRO:O | 1:D:1065:LEU:HD12 | 2.06 | 0.56 |
| 1:D:679:PHE:HZ | 1:D:684:LEU:HD12 | 1.69 | 0.56 |
| 1:F:945:ARG:NH1 | 1:F:1071:ILE:HG21 | 2.20 | 0.56 |
| 1:L:962:GLN:O | 1:L:966:GLU:HG3 | 2.06 | 0.56 |
| 1:I:969:LEU:HD23 | 1:L:873:HIS:CD2 | 2.41 | 0.56 |
| 1:C:909:ALA:HB2 | 1:C:917:ILE:HD11 | 1.88 | 0.56 |
| 1:C:679:PHE:HZ | 1:C:684:LEU:HD12 | 1.71 | 0.56 |
| 1:D:962:GLN:O | 1:D:966:GLU:HG3 | 2.05 | 0.56 |
| 1:L:941:PRO:O | 1:L:1065:LEU:HD12 | 2.05 | 0.56 |
| 1:K:935:LEU:O | 1:K:935:LEU:HD23 | 2.06 | 0.56 |
| 1:E:802:LEU:H | 1:E:802:LEU:HD22 | 1.70 | 0.56 |
| 1:H:732:ARG:HD2 | 1:H:825:HIS:O | 2.06 | 0.56 |
| 1:I:679:PHE:HZ | 1:I:684:LEU:HD12 | 1.71 | 0.56 |
| 1:G:845:ASN:HB3 | 1:H:887:ILE:HD13 | 1.88 | 0.56 |
| 1:G:754:THR:CG2 | 1:G:755:ARG:HH21 | 2.16 | 0.56 |
| 1:I:909:ALA:HB2 | 1:I:917:ILE:HD11 | 1.87 | 0.56 |
| 1:H:828:ARG:HG2 | 1:H:832:PHE:CG | 2.40 | 0.55 |
| 1:J:945:ARG:NH1 | 1:J:1071:ILE:HG21 | 2.21 | 0.55 |
| 1:D:862:TYR:OH | 1:D:869:ASN:ND2 | 2.38 | 0.55 |
| 1:C:1013:TRP:CE3 | 1:C:1057:ILE:HG22 | 2.40 | 0.55 |
| 1:L:660:ASP:O | 1:L:664:VAL:HG23 | 2.05 | 0.55 |
| 1:B:669:SER:HB3 | 1:B:673:LYS:NZ | 2.21 | 0.55 |
| 1:K:713:PHE:CD2 | 1:K:874:LEU:HD21 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C:935:LEU:O | 1:C:935:LEU:HD23 | 2.06 | 0.55 |
| 1:A:754:THR:CG2 | 1:A:755:ARG:HH21 | 2.17 | 0.55 |
| 1:L:751:TYR:CZ | 1:L:755:ARG:HG3 | 2.41 | 0.55 |
| 1:D:1003:TYR:CD2 | 1:D:1009:LEU:HG | 2.40 | 0.55 |
| 1:A:679:PHE:HZ | 1:A:684:LEU:HD12 | 1.71 | 0.55 |
| 1:I:730:GLY:HA3 | 1:I:823:TYR:HE1 | 1.68 | 0.55 |
| 1:D:751:TYR:CZ | 1:D:755:ARG:HG3 | 2.42 | 0.55 |
| 1:B:679:PHE:HZ | 1:B:684:LEU:HD12 | 1.71 | 0.55 |
| 1:J:941:PRO:O | 1:J:1065:LEU:HD12 | 2.06 | 0.55 |
| 1:C:1017:GLU:HB3 | 1:C:1055:ARG:HB2 | 1.88 | 0.55 |
| 1:G:708:GLY:O | 1:G:712:ILE:HG13 | 2.06 | 0.55 |
| 1:F:660:ASP:O | 1:F:664:VAL:HG23 | 2.07 | 0.55 |
| 1:F:828:ARG:HG2 | 1:F:832:PHE:CG | 2.42 | 0.55 |
| 1:A:730:GLY:HA3 | 1:A:823:TYR:HE1 | 1.66 | 0.55 |
| 1:D:825:HIS:CD2 | 1:D:827:GLY:H | 2.14 | 0.55 |
| 1:G:707:THR:CG2 | 1:G:709:LEU:HG | 2.37 | 0.55 |
| 1:I:719:GLN:HA | 1:I:722:ASN:HD22 | 1.70 | 0.55 |
| 1:B:828:ARG:HG2 | 1:B:832:PHE:CG | 2.41 | 0.55 |
| 1:C:751:TYR:CE2 | 1:C:755:ARG:HG3 | 2.42 | 0.55 |
| 1:L:945:ARG:NH1 | 1:L:1071:ILE:HG21 | 2.22 | 0.55 |
| 1:J:669:SER:HB3 | 1:J:673:LYS:NZ | 2.22 | 0.55 |
| 1:F:679:PHE:HZ | 1:F:684:LEU:HD12 | 1.72 | 0.55 |
| 1:K:760:LEU:HD23 | 1:K:801:CYS:N | 2.22 | 0.55 |
| 1:F:911:ASP:H | 1:F:914:SER:CB | 2.15 | 0.55 |
| 1:E:751:TYR:CZ | 1:E:755:ARG:HG3 | 2.42 | 0.55 |
| 1:A:802:LEU:H | 1:A:802:LEU:HD22 | 1.72 | 0.55 |
| 1:F:763:ILE:O | 1:F:764:HIS:CB | 2.53 | 0.55 |
| 1:H:700:MET:HE2 | 1:H:746:LEU:HD21 | 1.88 | 0.55 |
| 1:E:847:ARG:CZ | 1:F:891:LEU:HD13 | 2.37 | 0.55 |
| 1:H:962:GLN:O | 1:H:966:GLU:HG3 | 2.07 | 0.55 |
| 1:J:660:ASP:O | 1:J:664:VAL:HG23 | 2.07 | 0.55 |
| 1:B:748:ALA:HB3 | 1:B:936:ALA:HB1 | 1.89 | 0.55 |
| 1:B:1014:LEU:HD12 | 1:B:1056:ARG:CB | 2.36 | 0.55 |
| 1:B:881:ARG:HH11 | 1:B:881:ARG:HG3 | 1.72 | 0.55 |
| 1:E:708:GLY:O | 1:E:712:ILE:HG13 | 2.07 | 0.55 |
| 1:I:847:ARG:CZ | 1:J:891:LEU:HD13 | 2.37 | 0.55 |
| 1:A:718:GLN:HG3 | 1:A:722:ASN:HD21 | 1.71 | 0.55 |
| 1:K:802:LEU:HD22 | 1:K:802:LEU:H | 1.72 | 0.55 |
| 1:D:881:ARG:HH11 | 1:D:881:ARG:HG3 | 1.72 | 0.55 |
| 1:I:917:ILE:O | 1:I:918:GLU:HB2 | 2.05 | 0.54 |
| 1:J:862:TYR:OH | 1:J:869:ASN:ND2 | 2.40 | 0.54 |
| 1:G:842:VAL:HA | 1:H:883:ARG:HH22 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:D:737:HIS:HD2 | 1:D:958:GLU:OE2 | 1.90 | 0.54 |
| 1:B:862:TYR:OH | 1:B:869:ASN:ND2 | 2.37 | 0.54 |
| 1:G:945:ARG:HD3 | 1:L:915:ASN:HD21 | 1.72 | 0.54 |
| 1:C:754:THR:CG2 | 1:C:755:ARG:HH21 | 2.15 | 0.54 |
| 1:L:763:ILE:O | 1:L:764:HIS:CB | 2.55 | 0.54 |
| 1:C:825:HIS:HD2 | 1:C:827:GLY:N | 1.93 | 0.54 |
| 1:I:751:TYR:CE2 | 1:I:755:ARG:HG3 | 2.42 | 0.54 |
| 1:E:825:HIS:HD2 | 1:E:827:GLY:N | 1.93 | 0.54 |
| 1:G:751:TYR:CE2 | 1:G:755:ARG:HG3 | 2.41 | 0.54 |
| 1:A:751:TYR:CE2 | 1:A:755:ARG:HG3 | 2.42 | 0.54 |
| 1:D:945:ARG:NH1 | 1:D:1071:ILE:HG21 | 2.22 | 0.54 |
| 1:F:862:TYR:OH | 1:F:869:ASN:ND2 | 2.39 | 0.54 |
| 1:J:751:TYR:CZ | 1:J:755:ARG:HG3 | 2.42 | 0.54 |
| 1:H:862:TYR:OH | 1:H:869:ASN:ND2 | 2.39 | 0.54 |
| 1:A:721:MET:O | 1:A:725:ARG:HG3 | 2.08 | 0.54 |
| 1:I:708:GLY:O | 1:I:712:ILE:HG13 | 2.07 | 0.54 |
| 1:K:708:GLY:O | 1:K:712:ILE:HG13 | 2.08 | 0.54 |
| 1:E:762:GLN:HA | 1:E:805:ASN:HD21 | 1.73 | 0.54 |
| 1:K:847:ARG:CZ | 1:L:891:LEU:HD13 | 2.37 | 0.54 |
| 1:J:684:LEU:HD23 | 1:J:688:MET:HG3 | 1.89 | 0.54 |
| 1:G:935:LEU:HD23 | 1:G:935:LEU:O | 2.08 | 0.54 |
| 1:D:748:ALA:HB3 | 1:D:936:ALA:HB1 | 1.90 | 0.54 |
| 1:C:713:PHE:CD2 | 1:C:874:LEU:HD21 | 2.43 | 0.54 |
| 1:C:881:ARG:HG3 | 1:C:881:ARG:HH11 | 1.73 | 0.54 |
| 1:K:751:TYR:CE2 | 1:K:755:ARG:HG3 | 2.43 | 0.54 |
| 1:K:713:PHE:HD2 | 1:K:874:LEU:HD21 | 1.72 | 0.54 |
| 1:B:962:GLN:O | 1:B:966:GLU:HG3 | 2.07 | 0.54 |
| 1:D:660:ASP:O | 1:D:664:VAL:HG23 | 2.07 | 0.54 |
| 1:F:934:LYS:HD3 | 4:F:1335:HOH:O | 2.08 | 0.54 |
| 1:F:941:PRO:O | 1:F:1065:LEU:HD12 | 2.08 | 0.53 |
| 1:B:719:GLN:HE21 | 1:B:719:GLN:H | 0.79 | 0.53 |
| 1:L:735:PRO:HG2 | 1:L:958:GLU:HB2 | 1.90 | 0.53 |
| 1:L:684:LEU:HD23 | 1:L:688:MET:HG3 | 1.91 | 0.53 |
| 1:A:790:LYS:NZ | 1:J:1014:LEU:HD23 | 2.23 | 0.53 |
| 1:C:730:GLY:HA3 | 1:C:823:TYR:HE1 | 1.69 | 0.53 |
| 1:A:737:HIS:CD2 | 1:A:958:GLU:OE2 | 2.56 | 0.53 |
| 1:K:753:THR:HA | 1:K:802:LEU:HD23 | 1.90 | 0.53 |
| 1:J:761:GLN:HG2 | 1:J:763:ILE:H | 1.72 | 0.53 |
| 1:G:760:LEU:HD23 | 1:G:801:CYS:N | 2.23 | 0.53 |
| 1:L:862:TYR:OH | 1:L:869:ASN:ND2 | 2.39 | 0.53 |
| 1:F:751:TYR:CZ | 1:F:755:ARG:HG3 | 2.44 | 0.53 |
| 1:C:1017:GLU:CB | 1:C:1055:ARG:HD3 | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:H:737:HIS:HD2 | 1:H:958:GLU:OE2 | 1.91 | 0.53 |
| 1:B:945:ARG:NH1 | 1:B:1071:ILE:HG21 | 2.23 | 0.53 |
| 1:B:684:LEU:HD23 | 1:B:688:MET:HG3 | 1.89 | 0.53 |
| 1:I:765:ASN:HA | 1:I:804:SER:HB3 | 1.90 | 0.53 |
| 1:C:802:LEU:H | 1:C:802:LEU:HD22 | 1.73 | 0.53 |
| 1:C:708:GLY:O | 1:C:712:ILE:HG13 | 2.08 | 0.53 |
| 1:F:700:MET:HE2 | 1:F:746:LEU:CD2 | 2.39 | 0.53 |
| 1:J:748:ALA:HB3 | 1:J:936:ALA:HB1 | 1.90 | 0.53 |
| 1:I:721:MET:O | 1:I:725:ARG:HG3 | 2.08 | 0.53 |
| 1:H:941:PRO:O | 1:H:1065:LEU:HD12 | 2.08 | 0.53 |
| 1:B:911:ASP:H | 1:B:914:SER:CB | 2.14 | 0.53 |
| 1:E:730:GLY:HA3 | 1:E:823:TYR:HE1 | 1.69 | 0.53 |
| 1:L:732:ARG:HD2 | 1:L:825:HIS:O | 2.08 | 0.53 |
| 1:A:847:ARG:CZ | 1:B:891:LEU:HD13 | 2.39 | 0.53 |
| 1:H:915:ASN:HD21 | 1:K:945:ARG:CD | 2.22 | 0.53 |
| 1:J:1069:HIS:CE1 | 1:J:1073:LYS:HZ2 | 2.27 | 0.53 |
| 1:J:828:ARG:HG2 | 1:J:832:PHE:CG | 2.43 | 0.53 |
| 1:F:1059:CYS:HB3 | 1:F:1062:MET:CB | 2.38 | 0.53 |
| 1:H:1014:LEU:HD21 | 1:H:1058:PHE:HB2 | 1.91 | 0.53 |
| 1:F:735:PRO:HG2 | 1:F:958:GLU:HB2 | 1.91 | 0.53 |
| 1:J:679:PHE:HZ | 1:J:684:LEU:HD12 | 1.73 | 0.53 |
| 1:C:739:ARG:HG2 | 4:C:1223:HOH:O | 2.08 | 0.53 |
| 1:C:760:LEU:HD23 | 1:C:801:CYS:N | 2.24 | 0.53 |
| 1:H:881:ARG:HH11 | 1:H:881:ARG:HG3 | 1.72 | 0.53 |
| 1:C:751:TYR:CZ | 1:C:755:ARG:HG3 | 2.44 | 0.53 |
| 1:F:952:THR:HG23 | 1:F:988:GLN:NE2 | 2.24 | 0.53 |
| 1:J:704:PHE:HB3 | 1:J:710:LEU:HG | 1.91 | 0.53 |
| 1:G:881:ARG:HG3 | 1:G:881:ARG:HH11 | 1.74 | 0.53 |
| 1:A:719:GLN:HA | 1:A:722:ASN:HD22 | 1.73 | 0.53 |
| 1:G:753:THR:HA | 1:G:802:LEU:HD23 | 1.91 | 0.53 |
| 1:E:753:THR:HA | 1:E:802:LEU:HD23 | 1.91 | 0.53 |
| 1:J:763:ILE:O | 1:J:764:HIS:CB | 2.57 | 0.53 |
| 1:H:915:ASN:HD21 | 1:K:945:ARG:HD3 | 1.74 | 0.53 |
| 1:K:721:MET:O | 1:K:725:ARG:HG3 | 2.09 | 0.53 |
| 1:I:713:PHE:CD2 | 1:I:874:LEU:HD21 | 2.44 | 0.53 |
| 1:F:881:ARG:HH11 | 1:F:881:ARG:HG3 | 1.73 | 0.53 |
| 1:H:828:ARG:NH1 | 1:H:965:GLU:OE1 | 2.43 | 0.52 |
| 1:J:737:HIS:HD2 | 1:J:958:GLU:OE2 | 1.91 | 0.52 |
| 1:L:1069:HIS:CE1 | 1:L:1073:LYS:HZ2 | 2.27 | 0.52 |
| 1:J:1059:CYS:HB2 | 1:J:1062:MET:HB2 | 1.91 | 0.52 |
| 1:L:881:ARG:HH11 | 1:L:881:ARG:HG3 | 1.74 | 0.52 |
| 1:I:754:THR:HG22 | 1:I:755:ARG:NE | 2.21 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:F:685:VAL:HG22 | 1:F:695:ILE:CD1 | 2.39 | 0.52 |
| 1:A:909:ALA:HB2 | 1:A:917:ILE:HD11 | 1.89 | 0.52 |
| 1:C:1017:GLU:N | 1:C:1055:ARG:HD3 | 2.22 | 0.52 |
| 1:F:737:HIS:HD2 | 1:F:958:GLU:OE2 | 1.93 | 0.52 |
| 1:H:684:LEU:HD23 | 1:H:688:MET:HG3 | 1.92 | 0.52 |
| 1:D:762:GLN:HA | 1:D:762:GLN:OE1 | 2.10 | 0.52 |
| 1:E:1017:GLU:CB | 1:E:1055:ARG:HD3 | 2.38 | 0.52 |
| 1:F:1014:LEU:HD13 | 1:F:1056:ARG:NH2 | 2.25 | 0.52 |
| 1:D:828:ARG:HG2 | 1:D:832:PHE:CG | 2.43 | 0.52 |
| 1:L:737:HIS:HD2 | 1:L:958:GLU:OE2 | 1.92 | 0.52 |
| 1:E:763:ILE:H | 1:E:805:ASN:ND2 | 2.07 | 0.52 |
| 1:E:662:ILE:O | 1:E:666:GLU:HG3 | 2.08 | 0.52 |
| 1:G:751:TYR:CZ | 1:G:755:ARG:HG3 | 2.44 | 0.52 |
| 1:J:732:ARG:HD2 | 1:J:825:HIS:O | 2.10 | 0.52 |
| 1:I:891:LEU:CD1 | 1:J:847:ARG:NH2 | 2.70 | 0.52 |
| 1:K:707:THR:HG22 | 1:K:709:LEU:HG | 1.91 | 0.52 |
| 1:C:753:THR:HA | 1:C:802:LEU:HD23 | 1.91 | 0.52 |
| 1:E:713:PHE:CD2 | 1:E:874:LEU:HD21 | 2.45 | 0.52 |
| 1:B:737:HIS:HD2 | 1:B:958:GLU:OE2 | 1.93 | 0.52 |
| 1:C:1056:ARG:NH1 | 1:C:1056:ARG:HG3 | 2.25 | 0.52 |
| 1:L:704:PHE:HB3 | 1:L:710:LEU:HG | 1.92 | 0.52 |
| 1:D:684:LEU:HD23 | 1:D:688:MET:HG3 | 1.90 | 0.52 |
| 1:I:662:ILE:O | 1:I:666:GLU:HG3 | 2.10 | 0.52 |
| 1:F:804:SER:C | 1:F:805:ASN:HD22 | 2.13 | 0.52 |
| 1:A:707:THR:HG22 | 1:A:709:LEU:HG | 1.92 | 0.52 |
| 1:A:753:THR:HA | 1:A:802:LEU:HD23 | 1.92 | 0.52 |
| 1:J:911:ASP:H | 1:J:914:SER:CB | 2.15 | 0.51 |
| 1:D:1014:LEU:HD12 | 1:D:1056:ARG:CB | 2.40 | 0.51 |
| 1:B:915:ASN:HD21 | 1:C:945:ARG:HD3 | 1.75 | 0.51 |
| 1:H:915:ASN:CG | 1:K:945:ARG:NH1 | 2.63 | 0.51 |
| 1:B:674:MET:C | 1:B:676:ASN:H | 2.13 | 0.51 |
| 1:K:764:HIS:O | 1:K:766:GLY:N | 2.43 | 0.51 |
| 1:F:732:ARG:HD2 | 1:F:825:HIS:O | 2.11 | 0.51 |
| 1:C:1061:LEU:C | 1:C:1061:LEU:HD12 | 2.31 | 0.51 |
| 1:D:828:ARG:NH1 | 1:D:965:GLU:OE1 | 2.44 | 0.51 |
| 1:G:911:ASP:HB3 | 1:G:914:SER:CB | 2.41 | 0.51 |
| 1:D:804:SER:C | 1:D:805:ASN:HD22 | 2.13 | 0.51 |
| 1:J:881:ARG:HG3 | 1:J:881:ARG:HH11 | 1.75 | 0.51 |
| 1:J:1058:PHE:CD1 | 1:J:1063:HIS:CE1 | 2.98 | 0.51 |
| 1:G:721:MET:O | 1:G:725:ARG:HG3 | 2.10 | 0.51 |
| 1:A:1061:LEU:HD12 | 1:A:1061:LEU:C | 2.31 | 0.51 |
| 1:L:911:ASP:H | 1:L:914:SER:CB | 2.16 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:I:751:TYR:CZ | 1:I:755:ARG:HG3 | 2.46 | 0.51 |
| 1:C:1017:GLU:HB3 | 1:C:1055:ARG:CD | 2.41 | 0.51 |
| 1:E:1017:GLU:HB3 | 1:E:1055:ARG:CD | 2.41 | 0.51 |
| 1:E:760:LEU:HD23 | 1:E:801:CYS:N | 2.26 | 0.51 |
| 1:A:751:TYR:CZ | 1:A:755:ARG:HG3 | 2.45 | 0.51 |
| 1:D:732:ARG:HD2 | 1:D:825:HIS:O | 2.10 | 0.51 |
| 1:K:754:THR:CG2 | 1:K:755:ARG:HH21 | 2.18 | 0.51 |
| 1:I:737:HIS:CD2 | 1:I:958:GLU:OE2 | 2.56 | 0.51 |
| 1:D:704:PHE:HB3 | 1:D:710:LEU:HG | 1.91 | 0.51 |
| 1:A:935:LEU:HD23 | 1:A:935:LEU:O | 2.11 | 0.51 |
| 1:H:704:PHE:HB3 | 1:H:710:LEU:HG | 1.92 | 0.51 |
| 1:E:935:LEU:HD23 | 1:E:935:LEU:O | 2.11 | 0.51 |
| 1:K:881:ARG:HG3 | 1:K:881:ARG:HH11 | 1.76 | 0.51 |
| 1:E:881:ARG:HH11 | 1:E:881:ARG:HG3 | 1.76 | 0.51 |
| 1:I:753:THR:HA | 1:I:802:LEU:HD23 | 1.92 | 0.51 |
| 1:F:684:LEU:HD23 | 1:F:688:MET:HG3 | 1.92 | 0.51 |
| 1:K:911:ASP:HB3 | 1:K:914:SER:CB | 2.40 | 0.51 |
| 1:A:713:PHE:CD2 | 1:A:874:LEU:HD21 | 2.46 | 0.51 |
| 1:F:704:PHE:HB3 | 1:F:710:LEU:HG | 1.92 | 0.51 |
| 1:J:674:MET:C | 1:J:676:ASN:H | 2.13 | 0.51 |
| 1:C:721:MET:O | 1:C:725:ARG:HG3 | 2.10 | 0.51 |
| 1:C:713:PHE:HD2 | 1:C:874:LEU:HD21 | 1.76 | 0.51 |
| 1:F:674:MET:C | 1:F:676:ASN:H | 2.14 | 0.51 |
| 1:B:828:ARG:NH1 | 1:B:965:GLU:OE1 | 2.44 | 0.50 |
| 1:K:751:TYR:CZ | 1:K:755:ARG:HG3 | 2.45 | 0.50 |
| 1:L:674:MET:C | 1:L:676:ASN:H | 2.14 | 0.50 |
| 1:A:881:ARG:HG3 | 1:A:881:ARG:HH11 | 1.76 | 0.50 |
| 1:I:881:ARG:HG3 | 1:I:881:ARG:HH11 | 1.76 | 0.50 |
| 1:K:762:GLN:HA | 1:K:762:GLN:NE2 | 2.18 | 0.50 |
| 1:A:754:THR:HG22 | 1:A:755:ARG:NE | 2.22 | 0.50 |
| 1:D:763:ILE:O | 1:D:764:HIS:CB | 2.58 | 0.50 |
| 1:E:869:ASN:C | 1:E:869:ASN:HD22 | 2.14 | 0.50 |
| 1:B:952:THR:HG23 | 1:B:988:GLN:NE2 | 2.27 | 0.50 |
| 1:C:662:ILE:O | 1:C:666:GLU:HG3 | 2.10 | 0.50 |
| 1:A:708:GLY:O | 1:A:712:ILE:HG13 | 2.12 | 0.50 |
| 1:D:674:MET:C | 1:D:676:ASN:H | 2.13 | 0.50 |
| 1:H:685:VAL:HG22 | 1:H:695:ILE:CD1 | 2.41 | 0.50 |
| 1:J:685:VAL:HG22 | 1:J:695:ILE:CD1 | 2.41 | 0.50 |
| 1:E:1071:ILE:CG2 | 1:J:915:ASN:ND2 | 2.75 | 0.50 |
| 1:H:803:SER:HA | 1:H:811:LEU:HD11 | 1.94 | 0.50 |
| 1:A:1014:LEU:HD12 | 1:A:1056:ARG:CB | 2.42 | 0.50 |
| 1:D:735:PRO:HG2 | 1:D:958:GLU:HB2 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:735:PRO:HG2 | 1:B:958:GLU:HB2 | 1.94 | 0.50 |
| 1:E:713:PHE:HD2 | 1:E:874:LEU:HD21 | 1.77 | 0.50 |
| 1:L:1020:ASN:CG | 1:L:1021:ASP:H | 2.15 | 0.50 |
| 1:K:1061:LEU:C | 1:K:1061:LEU:HD12 | 2.31 | 0.50 |
| 1:H:674:MET:C | 1:H:676:ASN:H | 2.13 | 0.50 |
| 1:D:719:GLN:HE21 | 1:D:719:GLN:H | 0.81 | 0.50 |
| 1:F:828:ARG:NH1 | 1:F:965:GLU:OE1 | 2.44 | 0.50 |
| 1:J:739:ARG:CG | 1:J:739:ARG:HH11 | 2.23 | 0.50 |
| 1:L:735:PRO:HG2 | 1:L:958:GLU:CB | 2.41 | 0.50 |
| 1:J:735:PRO:HG2 | 1:J:958:GLU:HB2 | 1.92 | 0.50 |
| 1:L:976:PHE:CD2 | 1:L:987:LEU:HB2 | 2.47 | 0.50 |
| 1:L:828:ARG:NH1 | 1:L:965:GLU:OE1 | 2.45 | 0.50 |
| 1:L:964:ASP:OD2 | 1:L:979:ARG:NH1 | 2.45 | 0.50 |
| 1:A:911:ASP:HB3 | 1:A:914:SER:CB | 2.41 | 0.50 |
| 1:I:1061:LEU:HD12 | 1:I:1061:LEU:C | 2.32 | 0.50 |
| 1:D:965:GLU:O | 1:D:969:LEU:HG | 2.11 | 0.50 |
| 1:I:707:THR:HG22 | 1:I:709:LEU:HG | 1.94 | 0.50 |
| 1:F:761:GLN:HG2 | 1:F:763:ILE:H | 1.76 | 0.50 |
| 1:E:721:MET:O | 1:E:725:ARG:HG3 | 2.11 | 0.50 |
| 1:F:1013:TRP:CZ3 | 1:F:1055:ARG:HB3 | 2.47 | 0.50 |
| 1:C:869:ASN:HD22 | 1:C:869:ASN:C | 2.14 | 0.50 |
| 1:L:985:ALA:HA | 1:L:1072:TRP:CE3 | 2.47 | 0.50 |
| 1:D:911:ASP:H | 1:D:914:SER:CB | 2.18 | 0.50 |
| 1:G:730:GLY:HA3 | 1:G:823:TYR:HE1 | 1.68 | 0.50 |
| 1:C:891:LEU:HD13 | 1:D:847:ARG:NH2 | 2.26 | 0.50 |
| 1:C:911:ASP:HB3 | 1:C:914:SER:CB | 2.41 | 0.50 |
| 1:H:700:MET:HE3 | 1:H:746:LEU:CD1 | 2.42 | 0.50 |
| 1:K:660:ASP:O | 1:K:664:VAL:HG23 | 2.12 | 0.50 |
| 1:E:1061:LEU:HD12 | 1:E:1061:LEU:C | 2.32 | 0.50 |
| 1:H:911:ASP:H | 1:H:914:SER:CB | 2.16 | 0.49 |
| 1:C:737:HIS:CD2 | 1:C:958:GLU:OE2 | 2.58 | 0.49 |
| 1:J:684:LEU:HD23 | 1:J:684:LEU:O | 2.11 | 0.49 |
| 1:K:869:ASN:C | 1:K:869:ASN:HD22 | 2.15 | 0.49 |
| 1:H:763:ILE:O | 1:H:764:HIS:CB | 2.60 | 0.49 |
| 1:C:754:THR:HG22 | 1:C:755:ARG:NE | 2.21 | 0.49 |
| 1:A:662:ILE:O | 1:A:666:GLU:HG3 | 2.11 | 0.49 |
| 1:G:1061:LEU:HD12 | 1:G:1061:LEU:C | 2.33 | 0.49 |
| 1:H:761:GLN:HG2 | 1:H:763:ILE:H | 1.76 | 0.49 |
| 1:B:803:SER:HA | 1:B:811:LEU:HD11 | 1.93 | 0.49 |
| 1:J:804:SER:C | 1:J:805:ASN:HD22 | 2.15 | 0.49 |
| 1:E:739:ARG:HG2 | 4:E:1323:HOH:O | 2.11 | 0.49 |
| 1:I:869:ASN:C | 1:I:869:ASN:HD22 | 2.14 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:760:LEU:HD23 | 1:A:801:CYS:N | 2.27 | 0.49 |
| 1:C:754:THR:CG2 | 1:C:755:ARG:HE | 2.21 | 0.49 |
| 1:B:704:PHE:HB3 | 1:B:710:LEU:HG | 1.93 | 0.49 |
| 1:K:736:TYR:CD1 | 1:K:955:ILE:HG13 | 2.47 | 0.49 |
| 1:A:956:VAL:HG11 | 1:A:984:LEU:HD13 | 1.94 | 0.49 |
| 1:B:732:ARG:HD2 | 1:B:825:HIS:O | 2.12 | 0.49 |
| 1:I:713:PHE:HD2 | 1:I:874:LEU:HD21 | 1.76 | 0.49 |
| 1:G:713:PHE:CD2 | 1:G:874:LEU:HD21 | 2.48 | 0.49 |
| 1:B:1015:GLU:O | 1:B:1055:ARG:HD2 | 2.12 | 0.49 |
| 1:B:804:SER:C | 1:B:805:ASN:HD22 | 2.16 | 0.49 |
| 1:L:685:VAL:HG22 | 1:L:695:ILE:CD1 | 2.42 | 0.49 |
| 1:E:911:ASP:HB3 | 1:E:914:SER:CB | 2.42 | 0.49 |
| 1:H:700:MET:HE3 | 1:H:746:LEU:HD13 | 1.95 | 0.49 |
| 1:K:956:VAL:HG11 | 1:K:984:LEU:HD13 | 1.95 | 0.49 |
| 1:K:794:ASN:HB3 | 1:K:799:TYR:HB2 | 1.94 | 0.49 |
| 1:E:1059:CYS:SG | 1:E:1062:MET:HB2 | 2.53 | 0.49 |
| 1:I:911:ASP:HB3 | 1:I:914:SER:CB | 2.42 | 0.49 |
| 1:C:660:ASP:O | 1:C:664:VAL:HG23 | 2.13 | 0.49 |
| 1:L:803:SER:HA | 1:L:811:LEU:HD11 | 1.95 | 0.49 |
| 1:K:662:ILE:O | 1:K:666:GLU:HG3 | 2.12 | 0.49 |
| 1:H:804:SER:C | 1:H:805:ASN:HD22 | 2.16 | 0.49 |
| 1:A:736:TYR:CD1 | 1:A:955:ILE:HG13 | 2.48 | 0.49 |
| 1:G:660:ASP:O | 1:G:664:VAL:HG23 | 2.13 | 0.49 |
| 1:A:869:ASN:C | 1:A:869:ASN:HD22 | 2.16 | 0.49 |
| 1:I:935:LEU:O | 1:I:935:LEU:HD23 | 2.12 | 0.49 |
| 1:B:915:ASN:OD1 | 1:C:945:ARG:NH1 | 2.46 | 0.48 |
| 1:E:707:THR:HG22 | 1:E:709:LEU:HG | 1.94 | 0.48 |
| 1:D:1069:HIS:CE1 | 1:D:1073:LYS:HZ2 | 2.28 | 0.48 |
| 1:A:660:ASP:O | 1:A:664:VAL:HG23 | 2.13 | 0.48 |
| 1:C:736:TYR:CD1 | 1:C:955:ILE:HG13 | 2.48 | 0.48 |
| 1:B:810:GLU:OE1 | 1:B:925:ARG:HD2 | 2.13 | 0.48 |
| 1:F:1014:LEU:HD21 | 1:F:1058:PHE:HB2 | 1.95 | 0.48 |
| 1:B:685:VAL:HG22 | 1:B:695:ILE:CD1 | 2.43 | 0.48 |
| 1:K:729:ASN:HA | 1:K:739:ARG:NH2 | 2.27 | 0.48 |
| 1:D:934:LYS:HD3 | 4:D:1235:HOH:O | 2.14 | 0.48 |
| 1:C:816:VAL:O | 1:C:820:MET:HG2 | 2.13 | 0.48 |
| 1:J:1058:PHE:HE1 | 1:J:1063:HIS:CE1 | 2.30 | 0.48 |
| 1:A:729:ASN:HA | 1:A:739:ARG:NH2 | 2.28 | 0.48 |
| 1:D:700:MET:HE3 | 1:D:746:LEU:CD1 | 2.43 | 0.48 |
| 1:K:729:ASN:HA | 1:K:739:ARG:HH21 | 1.78 | 0.48 |
| 1:G:794:ASN:HB3 | 1:G:799:TYR:HB2 | 1.95 | 0.48 |
| 1:B:991:PHE:CE2 | 1:B:996:VAL:HG23 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:H:1069:HIS:CE1 | 1:H:1073:LYS:HZ2 | 2.29 | 0.48 |
| 1:G:662:ILE:O | 1:G:666:GLU:HG3 | 2.12 | 0.48 |
| 1:J:1058:PHE:CE1 | 1:J:1063:HIS:ND1 | 2.80 | 0.48 |
| 1:E:754:THR:CG2 | 1:E:755:ARG:HH21 | 2.18 | 0.48 |
| 1:B:964:ASP:OD2 | 1:B:979:ARG:NH1 | 2.46 | 0.48 |
| 1:F:735:PRO:HG2 | 1:F:958:GLU:CB | 2.44 | 0.48 |
| 1:C:956:VAL:HG11 | 1:C:984:LEU:HD13 | 1.94 | 0.48 |
| 1:C:846:ASP:OD2 | 1:D:883:ARG:NH1 | 2.47 | 0.48 |
| 1:F:965:GLU:O | 1:F:969:LEU:HG | 2.13 | 0.48 |
| 1:J:828:ARG:NH1 | 1:J:965:GLU:OE1 | 2.46 | 0.48 |
| 1:L:952:THR:HG23 | 1:L:988:GLN:NE2 | 2.28 | 0.48 |
| 1:D:685:VAL:HG22 | 1:D:695:ILE:CD1 | 2.43 | 0.48 |
| 1:C:707:THR:HG22 | 1:C:709:LEU:HG | 1.94 | 0.48 |
| 1:H:985:ALA:HA | 1:H:1072:TRP:CE3 | 2.49 | 0.48 |
| 1:J:965:GLU:O | 1:J:969:LEU:HG | 2.13 | 0.48 |
| 1:E:737:HIS:CD2 | 1:E:958:GLU:OE2 | 2.58 | 0.48 |
| 1:H:735:PRO:HG2 | 1:H:958:GLU:HB2 | 1.95 | 0.48 |
| 1:B:985:ALA:HA | 1:B:1072:TRP:CE3 | 2.49 | 0.48 |
| 1:D:803:SER:HA | 1:D:811:LEU:HD11 | 1.96 | 0.48 |
| 1:I:739:ARG:HG2 | 4:I:1523:HOH:O | 2.13 | 0.48 |
| 1:L:1059:CYS:HB3 | 1:L:1062:MET:HB2 | 1.96 | 0.48 |
| 1:H:716:PRO:HB2 | 1:H:719:GLN:HE22 | 1.79 | 0.48 |
| 1:G:825:HIS:HD2 | 1:G:827:GLY:N | 1.94 | 0.48 |
| 1:L:965:GLU:O | 1:L:969:LEU:HG | 2.14 | 0.48 |
| 1:F:964:ASP:OD2 | 1:F:979:ARG:NH1 | 2.47 | 0.48 |
| 1:G:847:ARG:CZ | 1:H:891:LEU:HD13 | 2.43 | 0.48 |
| 1:I:794:ASN:HB3 | 1:I:799:TYR:HB2 | 1.96 | 0.48 |
| 1:D:739:ARG:HH11 | 1:D:739:ARG:CG | 2.24 | 0.48 |
| 1:G:913:ASN:ND2 | 1:K:1056:ARG:HE | 2.12 | 0.48 |
| 1:H:964:ASP:OD2 | 1:H:979:ARG:NH1 | 2.47 | 0.48 |
| 1:G:945:ARG:NH1 | 1:L:918:GLU:OE2 | 2.47 | 0.48 |
| 1:C:1059:CYS:SG | 1:C:1062:MET:HB2 | 2.54 | 0.48 |
| 1:E:883:ARG:NH1 | 1:F:846:ASP:OD2 | 2.46 | 0.48 |
| 1:H:1013:TRP:CZ3 | 1:H:1057:ILE:HG22 | 2.48 | 0.47 |
| 1:C:763:ILE:C | 1:C:765:ASN:H | 2.17 | 0.47 |
| 1:I:736:TYR:CD1 | 1:I:955:ILE:HG13 | 2.49 | 0.47 |
| 1:H:952:THR:HG23 | 1:H:988:GLN:NE2 | 2.29 | 0.47 |
| 1:E:891:LEU:CD1 | 1:F:847:ARG:CZ | 2.93 | 0.47 |
| 1:E:891:LEU:HD13 | 1:F:847:ARG:NH2 | 2.28 | 0.47 |
| 1:E:1071:ILE:HG21 | 1:J:915:ASN:HD21 | 1.79 | 0.47 |
| 1:B:965:GLU:O | 1:B:969:LEU:HG | 2.14 | 0.47 |
| 1:H:729:ASN:HA | 1:H:739:ARG:HH22 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:I:762:GLN:HE22 | 1:I:801:CYS:H | 1.60 | 0.47 |
| 1:J:735:PRO:HG2 | 1:J:958:GLU:CB | 2.44 | 0.47 |
| 1:K:787:ILE:HG23 | 1:K:808:ALA:CB | 2.44 | 0.47 |
| 1:L:670:LEU:O | 1:L:674:MET:HG3 | 2.15 | 0.47 |
| 1:E:729:ASN:HA | 1:E:739:ARG:HH21 | 1.79 | 0.47 |
| 1:H:1059:CYS:HB3 | 1:H:1062:MET:HB2 | 1.96 | 0.47 |
| 1:H:991:PHE:CE2 | 1:H:996:VAL:HG23 | 2.49 | 0.47 |
| 1:A:724:PHE:O | 1:A:728:GLU:HG3 | 2.13 | 0.47 |
| 1:H:1056:ARG:NH1 | 1:H:1056:ARG:HB3 | 2.28 | 0.47 |
| 1:C:729:ASN:HA | 1:C:739:ARG:NH2 | 2.28 | 0.47 |
| 1:I:729:ASN:HA | 1:I:739:ARG:NH2 | 2.29 | 0.47 |
| 1:L:810:GLU:OE1 | 1:L:925:ARG:HD2 | 2.15 | 0.47 |
| 1:D:796:ASP:OD1 | 1:D:798:SER:N | 2.39 | 0.47 |
| 1:E:794:ASN:HB3 | 1:E:799:TYR:HB2 | 1.96 | 0.47 |
| 1:J:803:SER:HA | 1:J:811:LEU:HD11 | 1.96 | 0.47 |
| 1:G:754:THR:HG22 | 1:G:755:ARG:NE | 2.22 | 0.47 |
| 1:C:891:LEU:CD1 | 1:D:847:ARG:CZ | 2.92 | 0.47 |
| 1:H:735:PRO:HG2 | 1:H:958:GLU:CB | 2.45 | 0.47 |
| 1:D:700:MET:HE3 | 1:D:746:LEU:HD13 | 1.95 | 0.47 |
| 1:I:847:ARG:NH2 | 1:J:891:LEU:HD13 | 2.30 | 0.47 |
| 1:L:674:MET:HE3 | 1:L:699:VAL:HG13 | 1.97 | 0.47 |
| 1:D:716:PRO:HB2 | 1:D:719:GLN:HE22 | 1.80 | 0.47 |
| 1:I:760:LEU:HD23 | 1:I:801:CYS:N | 2.30 | 0.47 |
| 1:B:735:PRO:HG2 | 1:B:958:GLU:CB | 2.44 | 0.47 |
| 1:G:707:THR:HG22 | 1:G:709:LEU:HG | 1.97 | 0.47 |
| 1:E:846:ASP:HB2 | 4:E:1334:HOH:O | 2.14 | 0.47 |
| 1:D:735:PRO:HG2 | 1:D:958:GLU:CB | 2.44 | 0.47 |
| 1:I:729:ASN:HA | 1:I:739:ARG:HH21 | 1.79 | 0.47 |
| 1:J:810:GLU:OE1 | 1:J:925:ARG:HD2 | 2.14 | 0.47 |
| 1:K:727:LEU:HD21 | 1:K:820:MET:HB3 | 1.97 | 0.47 |
| 1:A:701:TYR:OH | 1:J:1015:GLU:OE1 | 2.32 | 0.47 |
| 1:E:952:THR:HG23 | 1:E:988:GLN:NE2 | 2.30 | 0.47 |
| 1:K:670:LEU:HD22 | 1:K:674:MET:SD | 2.54 | 0.47 |
| 1:G:796:ASP:OD1 | 1:G:798:SER:CB | 2.63 | 0.47 |
| 1:B:872:LEU:HD13 | 1:B:873:HIS:CG | 2.50 | 0.47 |
| 1:B:1014:LEU:HD21 | 1:B:1058:PHE:HB2 | 1.97 | 0.47 |
| 1:B:729:ASN:HA | 1:B:739:ARG:HH22 | 1.80 | 0.47 |
| 1:B:700:MET:HE3 | 1:B:746:LEU:HD13 | 1.97 | 0.47 |
| 1:C:729:ASN:HA | 1:C:739:ARG:HH21 | 1.78 | 0.47 |
| 1:A:1014:LEU:HD12 | 1:A:1056:ARG:HB3 | 1.97 | 0.47 |
| 1:D:964:ASP:OD2 | 1:D:979:ARG:NH1 | 2.47 | 0.47 |
| 1:B:684:LEU:HD23 | 1:B:684:LEU:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:L:985:ALA:HA | 1:L:1072:TRP:HE3 | 1.79 | 0.47 |
| 1:E:729:ASN:HA | 1:E:739:ARG:NH2 | 2.29 | 0.47 |
| 1:G:816:VAL:O | 1:G:820:MET:HG2 | 2.14 | 0.47 |
| 1:B:845:ASN:O | 1:B:847:ARG:HG2 | 2.15 | 0.47 |
| 1:B:981:SER:N | 1:B:982:PRO:CD | 2.78 | 0.47 |
| 1:A:729:ASN:HA | 1:A:739:ARG:HH21 | 1.79 | 0.47 |
| 1:J:700:MET:HE3 | 1:J:746:LEU:CD1 | 2.45 | 0.47 |
| 1:E:816:VAL:O | 1:E:820:MET:HG2 | 2.15 | 0.47 |
| 1:C:794:ASN:HB3 | 1:C:799:TYR:HB2 | 1.97 | 0.47 |
| 1:J:985:ALA:HA | 1:J:1072:TRP:CE3 | 2.50 | 0.47 |
| 1:D:985:ALA:HA | 1:D:1072:TRP:CE3 | 2.49 | 0.47 |
| 1:D:1057:ILE:HD12 | 1:D:1058:PHE:N | 2.30 | 0.46 |
| 1:G:1056:ARG:HH11 | 1:G:1056:ARG:HG3 | 1.80 | 0.46 |
| 1:J:719:GLN:H | 1:J:719:GLN:HE21 | 0.80 | 0.46 |
| 1:E:754:THR:HG22 | 1:E:755:ARG:NE | 2.24 | 0.46 |
| 1:B:700:MET:HE3 | 1:B:746:LEU:CD1 | 2.46 | 0.46 |
| 1:E:956:VAL:HG11 | 1:E:984:LEU:HD13 | 1.97 | 0.46 |
| 1:G:670:LEU:HD22 | 1:G:674:MET:SD | 2.55 | 0.46 |
| 1:H:965:GLU:O | 1:H:969:LEU:HG | 2.15 | 0.46 |
| 1:L:729:ASN:HA | 1:L:739:ARG:HH22 | 1.80 | 0.46 |
| 1:G:729:ASN:HA | 1:G:739:ARG:NH2 | 2.31 | 0.46 |
| 1:A:1056:ARG:HH11 | 1:A:1056:ARG:HG3 | 1.80 | 0.46 |
| 1:F:1069:HIS:ND1 | 1:F:1073:LYS:NZ | 2.56 | 0.46 |
| 1:I:1056:ARG:NH1 | 1:I:1056:ARG:HG3 | 2.31 | 0.46 |
| 1:I:869:ASN:C | 1:I:869:ASN:ND2 | 2.69 | 0.46 |
| 1:G:674:MET:CE | 1:G:703:LEU:HD21 | 2.45 | 0.46 |
| 1:L:991:PHE:CE2 | 1:L:996:VAL:HG23 | 2.50 | 0.46 |
| 1:L:804:SER:C | 1:L:805:ASN:HD22 | 2.19 | 0.46 |
| 1:I:670:LEU:HD22 | 1:I:674:MET:SD | 2.56 | 0.46 |
| 1:D:930:GLN:O | 1:D:933:ILE:HG13 | 2.16 | 0.46 |
| 1:A:1017:GLU:HB3 | 1:A:1055:ARG:CD | 2.46 | 0.46 |
| 1:B:915:ASN:OD1 | 1:C:945:ARG:CZ | 2.64 | 0.46 |
| 1:H:845:ASN:O | 1:H:847:ARG:HG2 | 2.15 | 0.46 |
| 1:H:981:SER:N | 1:H:982:PRO:CD | 2.79 | 0.46 |
| 1:E:869:ASN:ND2 | 1:E:869:ASN:C | 2.68 | 0.46 |
| 1:C:869:ASN:C | 1:C:869:ASN:ND2 | 2.69 | 0.46 |
| 1:G:727:LEU:HD21 | 1:G:820:MET:HB3 | 1.97 | 0.46 |
| 1:J:938:ILE:HD12 | 1:J:996:VAL:HG22 | 1.97 | 0.46 |
| 1:K:823:TYR:CE2 | 1:K:857:SER:HB3 | 2.51 | 0.46 |
| 1:F:700:MET:CE | 1:F:746:LEU:CD2 | 2.94 | 0.46 |
| 1:E:1071:ILE:CG2 | 1:J:915:ASN:HD22 | 2.29 | 0.46 |
| 1:B:985:ALA:HA | 1:B:1072:TRP:HE3 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:E:846:ASP:OD2 | 1:F:883:ARG:NH1 | 2.48 | 0.46 |
| 1:F:976:PHE:CD2 | 1:F:987:LEU:HB2 | 2.50 | 0.46 |
| 1:I:660:ASP:O | 1:I:664:VAL:HG23 | 2.15 | 0.46 |
| 1:L:796:ASP:OD1 | 1:L:798:SER:N | 2.43 | 0.46 |
| 1:F:729:ASN:HA | 1:F:739:ARG:HH22 | 1.81 | 0.46 |
| 1:C:1017:GLU:H | 1:C:1055:ARG:CD | 2.27 | 0.46 |
| 1:A:939:ASN:ND2 | 1:A:943:LYS:HE3 | 2.31 | 0.46 |
| 1:J:952:THR:HG23 | 1:J:988:GLN:NE2 | 2.31 | 0.46 |
| 1:E:787:ILE:HG23 | 1:E:808:ALA:CB | 2.46 | 0.46 |
| 1:L:725:ARG:NH1 | 1:L:725:ARG:HG3 | 2.30 | 0.46 |
| 1:B:974:SER:HB2 | 1:B:977:MET:SD | 2.56 | 0.46 |
| 1:L:1014:LEU:HD21 | 1:L:1058:PHE:HB2 | 1.97 | 0.46 |
| 1:D:872:LEU:HD13 | 1:D:873:HIS:CG | 2.51 | 0.46 |
| 1:G:1056:ARG:HE | 1:K:913:ASN:ND2 | 2.13 | 0.46 |
| 1:K:707:THR:HG21 | 1:K:709:LEU:HG | 1.98 | 0.46 |
| 1:B:716:PRO:HB2 | 1:B:719:GLN:HE22 | 1.81 | 0.46 |
| 1:K:869:ASN:C | 1:K:869:ASN:ND2 | 2.70 | 0.46 |
| 1:H:872:LEU:HD13 | 1:H:873:HIS:CG | 2.51 | 0.46 |
| 1:L:973:ILE:HG21 | 1:L:978:ASP:HB2 | 1.97 | 0.46 |
| 1:J:976:PHE:CD2 | 1:J:987:LEU:HB2 | 2.51 | 0.46 |
| 1:A:718:GLN:OE1 | 1:J:1021:ASP:HA | 2.16 | 0.45 |
| 1:D:754:THR:CG2 | 1:D:755:ARG:HH21 | 2.26 | 0.45 |
| 1:F:754:THR:CG2 | 1:F:755:ARG:HH21 | 2.25 | 0.45 |
| 1:J:725:ARG:NH1 | 1:J:725:ARG:HG3 | 2.31 | 0.45 |
| 1:F:981:SER:N | 1:F:982:PRO:CD | 2.79 | 0.45 |
| 1:K:871:LEU:HB3 | 1:K:874:LEU:HD12 | 1.98 | 0.45 |
| 1:K:846:ASP:HB2 | 4:K:1634:HOH:O | 2.15 | 0.45 |
| 1:I:956:VAL:HG11 | 1:I:984:LEU:HD13 | 1.97 | 0.45 |
| 1:G:736:TYR:CD1 | 1:G:955:ILE:HG13 | 2.50 | 0.45 |
| 1:D:973:ILE:HG21 | 1:D:978:ASP:HB2 | 1.98 | 0.45 |
| 1:B:915:ASN:HD21 | 1:C:945:ARG:HD2 | 1.81 | 0.45 |
| 1:H:1057:ILE:HD12 | 1:H:1058:PHE:N | 2.31 | 0.45 |
| 1:I:816:VAL:O | 1:I:820:MET:HG2 | 2.16 | 0.45 |
| 1:D:1020:ASN:HA | 1:D:1020:ASN:HD22 | 1.59 | 0.45 |
| 1:K:754:THR:CG2 | 1:K:755:ARG:HE | 2.21 | 0.45 |
| 1:E:754:THR:CG2 | 1:E:755:ARG:HE | 2.24 | 0.45 |
| 1:D:1069:HIS:ND1 | 1:D:1073:LYS:NZ | 2.54 | 0.45 |
| 1:A:727:LEU:HD21 | 1:A:820:MET:HB3 | 1.99 | 0.45 |
| 1:A:816:VAL:O | 1:A:820:MET:HG2 | 2.15 | 0.45 |
| 1:G:945:ARG:CD | 1:L:915:ASN:HD21 | 2.28 | 0.45 |
| 1:K:816:VAL:O | 1:K:820:MET:HG2 | 2.16 | 0.45 |
| 1:F:985:ALA:HA | 1:F:1072:TRP:CE3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:D:810:GLU:OE1 | 1:D:925:ARG:HD2 | 2.16 | 0.45 |
| 1:D:703:LEU:HD22 | 1:D:750:TRP:CE2 | 2.52 | 0.45 |
| 1:G:939:ASN:ND2 | 1:G:943:LYS:HE3 | 2.32 | 0.45 |
| 1:D:1014:LEU:HD12 | 1:D:1056:ARG:HB2 | 1.96 | 0.45 |
| 1:B:915:ASN:CG | 1:C:945:ARG:HH11 | 2.14 | 0.45 |
| 1:G:787:ILE:HG23 | 1:G:808:ALA:CB | 2.47 | 0.45 |
| 1:A:707:THR:HG21 | 1:A:709:LEU:HG | 1.98 | 0.45 |
| 1:F:674:MET:HE3 | 1:F:699:VAL:HG13 | 1.99 | 0.45 |
| 1:K:674:MET:CE | 1:K:703:LEU:HD21 | 2.47 | 0.45 |
| 1:G:956:VAL:HG11 | 1:G:984:LEU:HD13 | 1.98 | 0.45 |
| 1:B:976:PHE:CD2 | 1:B:987:LEU:HB2 | 2.51 | 0.45 |
| 1:F:1014:LEU:HD12 | 1:F:1056:ARG:HB3 | 1.99 | 0.45 |
| 1:J:700:MET:HE3 | 1:J:746:LEU:HD13 | 1.99 | 0.45 |
| 1:D:700:MET:CE | 1:D:746:LEU:CD2 | 2.94 | 0.45 |
| 1:H:725:ARG:HG3 | 1:H:725:ARG:NH1 | 2.30 | 0.45 |
| 1:A:713:PHE:HD2 | 1:A:874:LEU:HD21 | 1.81 | 0.45 |
| 1:J:670:LEU:O | 1:J:674:MET:HG3 | 2.17 | 0.45 |
| 1:D:674:MET:HE3 | 1:D:699:VAL:HG13 | 1.98 | 0.45 |
| 1:L:938:ILE:HD12 | 1:L:996:VAL:HG22 | 1.97 | 0.45 |
| 1:E:660:ASP:O | 1:E:664:VAL:HG23 | 2.17 | 0.45 |
| 1:A:957:ASN:O | 1:A:961:GLU:HG3 | 2.16 | 0.45 |
| 1:F:719:GLN:H | 1:F:719:GLN:HE21 | 0.79 | 0.45 |
| 1:F:739:ARG:HH11 | 1:F:739:ARG:CG | 2.26 | 0.45 |
| 1:C:764:HIS:O | 1:C:765:ASN:O | 2.35 | 0.45 |
| 1:B:872:LEU:HD13 | 1:B:873:HIS:CD2 | 2.52 | 0.45 |
| 1:E:957:ASN:O | 1:E:961:GLU:HG3 | 2.17 | 0.45 |
| 1:D:938:ILE:HD12 | 1:D:996:VAL:HG22 | 1.98 | 0.45 |
| 1:H:851:GLU:HA | 1:H:854:HIS:HD2 | 1.82 | 0.45 |
| 1:D:1055:ARG:HG2 | 1:D:1056:ARG:H | 1.81 | 0.45 |
| 1:C:787:ILE:HG23 | 1:C:808:ALA:CB | 2.47 | 0.45 |
| 1:J:1059:CYS:HB2 | 1:J:1062:MET:CB | 2.47 | 0.45 |
| 1:B:670:LEU:O | 1:B:674:MET:HG3 | 2.16 | 0.45 |
| 1:H:976:PHE:CD2 | 1:H:987:LEU:HB2 | 2.51 | 0.45 |
| 1:C:784:ILE:HG21 | 1:C:807:PRO:HB3 | 1.97 | 0.45 |
| 1:B:703:LEU:HD22 | 1:B:750:TRP:CE2 | 2.52 | 0.45 |
| 1:A:762:GLN:NE2 | 1:A:800:GLY:HA2 | 2.31 | 0.45 |
| 1:B:694:ARG:O | 1:B:698:GLN:HG2 | 2.17 | 0.45 |
| 1:B:700:MET:CE | 1:B:746:LEU:CD2 | 2.95 | 0.45 |
| 1:H:985:ALA:HA | 1:H:1072:TRP:HE3 | 1.81 | 0.45 |
| 1:J:754:THR:CG2 | 1:J:755:ARG:HH21 | 2.26 | 0.45 |
| 1:L:694:ARG:O | 1:L:698:GLN:HG2 | 2.17 | 0.45 |
| 1:A:869:ASN:C | 1:A:869:ASN:ND2 | 2.71 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:F:851:GLU:HA | 1:F:854:HIS:HD2 | 1.81 | 0.45 |
| 1:E:784:ILE:HG22 | 1:E:786:TYR:CE1 | 2.52 | 0.45 |
| 1:F:796:ASP:OD1 | 1:F:798:SER:N | 2.41 | 0.45 |
| 1:G:1056:ARG:HH21 | 1:K:913:ASN:HD22 | 1.65 | 0.44 |
| 1:I:724:PHE:O | 1:I:728:GLU:HG3 | 2.16 | 0.44 |
| 1:F:700:MET:HE3 | 1:F:746:LEU:HD13 | 1.99 | 0.44 |
| 1:L:981:SER:N | 1:L:982:PRO:CD | 2.79 | 0.44 |
| 1:E:763:ILE:H | 1:E:805:ASN:HD21 | 1.64 | 0.44 |
| 1:B:705:GLN:HG2 | 1:B:710:LEU:HD12 | 1.99 | 0.44 |
| 1:J:872:LEU:HD13 | 1:J:873:HIS:CG | 2.52 | 0.44 |
| 1:E:796:ASP:OD1 | 1:E:798:SER:CB | 2.66 | 0.44 |
| 1:B:851:GLU:HA | 1:B:854:HIS:HD2 | 1.82 | 0.44 |
| 1:C:707:THR:HG21 | 1:C:709:LEU:HG | 1.98 | 0.44 |
| 1:I:915:ASN:HD22 | 1:I:915:ASN:HA | 1.65 | 0.44 |
| 1:L:705:GLN:HG2 | 1:L:710:LEU:HD12 | 1.99 | 0.44 |
| 1:C:670:LEU:HD22 | 1:C:674:MET:SD | 2.57 | 0.44 |
| 1:I:823:TYR:CE2 | 1:I:857:SER:HB3 | 2.52 | 0.44 |
| 1:D:845:ASN:O | 1:D:847:ARG:HG2 | 2.17 | 0.44 |
| 1:G:913:ASN:ND2 | 1:K:1056:ARG:NH2 | 2.60 | 0.44 |
| 1:J:694:ARG:O | 1:J:698:GLN:HG2 | 2.17 | 0.44 |
| 1:B:725:ARG:HG3 | 1:B:725:ARG:NH1 | 2.30 | 0.44 |
| 1:K:846:ASP:OD2 | 1:L:883:ARG:NH1 | 2.51 | 0.44 |
| 1:E:939:ASN:ND2 | 1:E:943:LYS:HE3 | 2.33 | 0.44 |
| 1:L:930:GLN:O | 1:L:933:ILE:HG13 | 2.17 | 0.44 |
| 1:J:973:ILE:HG21 | 1:J:978:ASP:HB2 | 1.99 | 0.44 |
| 1:G:823:TYR:CE2 | 1:G:857:SER:HB3 | 2.53 | 0.44 |
| 1:D:694:ARG:O | 1:D:698:GLN:HG2 | 2.17 | 0.44 |
| 1:G:674:MET:HE1 | 1:G:703:LEU:HD21 | 2.00 | 0.44 |
| 1:C:847:ARG:CZ | 1:D:891:LEU:HD13 | 2.48 | 0.44 |
| 1:E:823:TYR:CE2 | 1:E:857:SER:HB3 | 2.52 | 0.44 |
| 1:J:1003:TYR:HD2 | 1:J:1009:LEU:HG | 1.81 | 0.44 |
| 1:D:981:SER:N | 1:D:982:PRO:CD | 2.79 | 0.44 |
| 1:F:684:LEU:O | 1:F:684:LEU:HD23 | 2.17 | 0.44 |
| 1:B:963:GLY:O | 1:B:973:ILE:HD12 | 2.18 | 0.44 |
| 1:G:762:GLN:HB3 | 1:G:765:ASN:CB | 2.47 | 0.44 |
| 1:K:724:PHE:O | 1:K:728:GLU:HG3 | 2.17 | 0.44 |
| 1:L:721:MET:O | 1:L:725:ARG:HG2 | 2.18 | 0.44 |
| 1:C:952:THR:O | 1:C:956:VAL:HG22 | 2.18 | 0.44 |
| 1:E:727:LEU:HD21 | 1:E:820:MET:HB3 | 2.00 | 0.44 |
| 1:I:957:ASN:O | 1:I:961:GLU:HG3 | 2.18 | 0.44 |
| 1:I:872:LEU:HD13 | 1:I:873:HIS:CD2 | 2.53 | 0.44 |
| 1:L:905:PHE:CD1 | 1:L:931:VAL:HG21 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:814:LEU:HD11 | 1:A:933:ILE:HB | 2.00 | 0.44 |
| 1:D:729:ASN:HA | 1:D:739:ARG:HH22 | 1.82 | 0.44 |
| 1:B:739:ARG:HH11 | 1:B:739:ARG:CG | 2.23 | 0.44 |
| 1:H:751:TYR:CE2 | 1:H:755:ARG:HG3 | 2.52 | 0.44 |
| 1:A:787:ILE:HG23 | 1:A:808:ALA:CB | 2.48 | 0.44 |
| 1:D:684:LEU:O | 1:D:684:LEU:HD23 | 2.18 | 0.44 |
| 1:E:847:ARG:NH2 | 1:F:891:LEU:HD13 | 2.33 | 0.44 |
| 1:C:939:ASN:ND2 | 1:C:943:LYS:HE3 | 2.33 | 0.44 |
| 1:G:869:ASN:HD22 | 1:G:869:ASN:C | 2.20 | 0.44 |
| 1:H:694:ARG:O | 1:H:698:GLN:HG2 | 2.18 | 0.44 |
| 1:J:845:ASN:O | 1:J:847:ARG:HG2 | 2.17 | 0.44 |
| 1:G:729:ASN:HA | 1:G:739:ARG:HH21 | 1.82 | 0.44 |
| 1:G:915:ASN:HD22 | 1:G:915:ASN:HA | 1.65 | 0.44 |
| 1:H:721:MET:O | 1:H:725:ARG:HG2 | 2.18 | 0.44 |
| 1:H:1004:ASP:HA | 1:H:1009:LEU:HD12 | 1.99 | 0.44 |
| 1:D:670:LEU:O | 1:D:674:MET:HG3 | 2.18 | 0.44 |
| 1:I:872:LEU:HD13 | 1:I:873:HIS:CG | 2.53 | 0.44 |
| 1:F:803:SER:HA | 1:F:811:LEU:HD11 | 1.99 | 0.44 |
| 1:H:974:SER:HB2 | 1:H:977:MET:SD | 2.58 | 0.44 |
| 1:D:976:PHE:CD2 | 1:D:987:LEU:HB2 | 2.53 | 0.44 |
| 1:A:670:LEU:HD22 | 1:A:674:MET:SD | 2.58 | 0.44 |
| 1:A:674:MET:CE | 1:A:703:LEU:HD21 | 2.48 | 0.44 |
| 1:K:764:HIS:O | 1:K:804:SER:O | 2.36 | 0.44 |
| 1:H:825:HIS:CD2 | 1:H:826:PRO:HD2 | 2.53 | 0.44 |
| 1:L:681:ILE:H | 1:L:681:ILE:HG13 | 1.45 | 0.44 |
| 1:J:964:ASP:OD2 | 1:J:979:ARG:NH1 | 2.51 | 0.44 |
| 1:J:981:SER:N | 1:J:982:PRO:CD | 2.79 | 0.44 |
| 1:F:805:ASN:N | 1:F:805:ASN:HD22 | 2.16 | 0.44 |
| 1:G:957:ASN:O | 1:G:961:GLU:HG3 | 2.17 | 0.44 |
| 1:F:810:GLU:OE1 | 1:F:925:ARG:HD2 | 2.18 | 0.44 |
| 1:F:930:GLN:O | 1:F:933:ILE:HG13 | 2.18 | 0.44 |
| 1:J:796:ASP:OD1 | 1:J:798:SER:N | 2.41 | 0.44 |
| 1:E:891:LEU:HD12 | 1:F:847:ARG:CZ | 2.48 | 0.43 |
| 1:G:724:PHE:O | 1:G:728:GLU:HG3 | 2.17 | 0.43 |
| 1:L:956:VAL:HG23 | 1:L:957:ASN:N | 2.33 | 0.43 |
| 1:I:707:THR:HG21 | 1:I:709:LEU:HG | 1.99 | 0.43 |
| 1:L:872:LEU:HD13 | 1:L:873:HIS:CG | 2.53 | 0.43 |
| 1:G:713:PHE:HD2 | 1:G:874:LEU:HD21 | 1.82 | 0.43 |
| 1:F:973:ILE:HG21 | 1:F:978:ASP:HB2 | 1.98 | 0.43 |
| 1:E:872:LEU:HD13 | 1:E:873:HIS:CG | 2.53 | 0.43 |
| 1:F:872:LEU:HD13 | 1:F:873:HIS:CG | 2.53 | 0.43 |
| 1:I:754:THR:CG2 | 1:I:755:ARG:HE | 2.21 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:847:ARG:NH2 | 1:B:891:LEU:HD13 | 2.32 | 0.43 |
| 1:L:670:LEU:HD22 | 1:L:674:MET:SD | 2.58 | 0.43 |
| 1:D:985:ALA:HA | 1:D:1072:TRP:HE3 | 1.82 | 0.43 |
| 1:J:991:PHE:CE2 | 1:J:996:VAL:HG23 | 2.54 | 0.43 |
| 1:G:765:ASN:HA | 1:G:804:SER:HB3 | 2.00 | 0.43 |
| 1:K:1004:ASP:CB | 1:K:1009:LEU:HD12 | 2.48 | 0.43 |
| 1:L:959:PHE:HA | 1:L:977:MET:HE2 | 2.00 | 0.43 |
| 1:K:939:ASN:ND2 | 1:K:943:LYS:HE3 | 2.33 | 0.43 |
| 1:J:729:ASN:HA | 1:J:739:ARG:HH22 | 1.83 | 0.43 |
| 1:A:914:SER:OG | 1:A:915:ASN:N | 2.51 | 0.43 |
| 1:E:917:ILE:O | 1:E:924:ASP:OD2 | 2.36 | 0.43 |
| 1:D:725:ARG:HG3 | 1:D:725:ARG:NH1 | 2.32 | 0.43 |
| 1:B:881:ARG:HG3 | 1:B:881:ARG:NH1 | 2.33 | 0.43 |
| 1:J:670:LEU:HD22 | 1:J:674:MET:SD | 2.58 | 0.43 |
| 1:H:810:GLU:OE1 | 1:H:925:ARG:HD2 | 2.18 | 0.43 |
| 1:L:885:LEU:HA | 1:L:885:LEU:HD12 | 1.78 | 0.43 |
| 1:F:700:MET:HE3 | 1:F:746:LEU:CD1 | 2.48 | 0.43 |
| 1:B:694:ARG:HA | 1:B:728:GLU:OE2 | 2.18 | 0.43 |
| 1:L:963:GLY:O | 1:L:973:ILE:HD12 | 2.18 | 0.43 |
| 1:H:930:GLN:O | 1:H:933:ILE:HG13 | 2.17 | 0.43 |
| 1:J:851:GLU:HA | 1:J:854:HIS:HD2 | 1.83 | 0.43 |
| 1:K:952:THR:HG23 | 1:K:988:GLN:NE2 | 2.34 | 0.43 |
| 1:C:891:LEU:HD12 | 1:D:847:ARG:CZ | 2.49 | 0.43 |
| 1:D:1004:ASP:HA | 1:D:1009:LEU:HD12 | 2.00 | 0.43 |
| 1:D:881:ARG:NH1 | 1:D:881:ARG:HG3 | 2.34 | 0.43 |
| 1:C:842:VAL:HA | 1:D:883:ARG:HH22 | 1.83 | 0.43 |
| 1:H:872:LEU:HD13 | 1:H:873:HIS:CD2 | 2.53 | 0.43 |
| 1:F:985:ALA:HA | 1:F:1072:TRP:HE3 | 1.84 | 0.43 |
| 1:C:677:TRP:NE1 | 1:C:943:LYS:HD3 | 2.34 | 0.43 |
| 1:L:974:SER:HB2 | 1:L:977:MET:SD | 2.58 | 0.43 |
| 1:E:1013:TRP:CE3 | 1:E:1057:ILE:HG22 | 2.53 | 0.43 |
| 1:F:694:ARG:HA | 1:F:728:GLU:OE2 | 2.18 | 0.43 |
| 1:F:694:ARG:O | 1:F:698:GLN:HG2 | 2.17 | 0.43 |
| 1:B:956:VAL:HG23 | 1:B:957:ASN:N | 2.34 | 0.43 |
| 1:G:914:SER:OG | 1:G:915:ASN:N | 2.49 | 0.43 |
| 1:A:790:LYS:HZ3 | 1:J:1014:LEU:HD23 | 1.82 | 0.43 |
| 1:G:964:ASP:OD2 | 1:G:979:ARG:NH1 | 2.52 | 0.43 |
| 1:C:853:HIS:O | 1:C:857:SER:HB2 | 2.19 | 0.43 |
| 1:C:823:TYR:CE2 | 1:C:857:SER:HB3 | 2.53 | 0.43 |
| 1:D:754:THR:HG22 | 1:D:755:ARG:NE | 2.31 | 0.43 |
| 1:E:724:PHE:O | 1:E:728:GLU:HG3 | 2.18 | 0.43 |
| 1:H:956:VAL:HG23 | 1:H:957:ASN:N | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:I:787:ILE:HG23 | 1:I:808:ALA:CB | 2.48 | 0.43 |
| 1:L:758:PRO:HG3 | 1:L:799:TYR:HE2 | 1.84 | 0.43 |
| 1:J:700:MET:CE | 1:J:746:LEU:CD2 | 2.97 | 0.43 |
| 1:L:684:LEU:O | 1:L:684:LEU:HD23 | 2.19 | 0.43 |
| 1:B:670:LEU:HD22 | 1:B:674:MET:SD | 2.58 | 0.43 |
| 1:G:952:THR:HG23 | 1:G:988:GLN:NE2 | 2.34 | 0.43 |
| 1:E:677:TRP:NE1 | 1:E:943:LYS:HD3 | 2.33 | 0.43 |
| 1:E:939:ASN:O | 1:E:940:GLY:C | 2.57 | 0.43 |
| 1:I:803:SER:HA | 1:I:811:LEU:HD11 | 2.00 | 0.43 |
| 1:G:758:PRO:HD3 | 1:G:1011:GLY:H | 1.83 | 0.43 |
| 1:K:803:SER:HA | 1:K:811:LEU:HD11 | 2.01 | 0.43 |
| 1:D:956:VAL:HG23 | 1:D:957:ASN:N | 2.33 | 0.43 |
| 1:L:700:MET:HE2 | 1:L:746:LEU:CD2 | 2.47 | 0.43 |
| 1:I:914:SER:OG | 1:I:915:ASN:N | 2.51 | 0.43 |
| 1:H:684:LEU:O | 1:H:684:LEU:HD23 | 2.19 | 0.43 |
| 1:F:721:MET:O | 1:F:725:ARG:HG2 | 2.18 | 0.43 |
| 1:K:847:ARG:NH2 | 1:L:891:LEU:HD13 | 2.33 | 0.43 |
| 1:J:1069:HIS:ND1 | 1:J:1073:LYS:NZ | 2.54 | 0.43 |
| 1:D:805:ASN:HD22 | 1:D:805:ASN:N | 2.16 | 0.43 |
| 1:G:677:TRP:NE1 | 1:G:943:LYS:HD3 | 2.34 | 0.43 |
| 1:H:959:PHE:HA | 1:H:977:MET:HE2 | 1.99 | 0.43 |
| 1:H:723:TYR:CE1 | 1:H:861:LEU:HD13 | 2.53 | 0.43 |
| 1:F:681:ILE:H | 1:F:681:ILE:HG13 | 1.45 | 0.43 |
| 1:A:823:TYR:CE2 | 1:A:857:SER:HB3 | 2.54 | 0.43 |
| 1:C:724:PHE:O | 1:C:728:GLU:HG3 | 2.19 | 0.43 |
| 1:B:755:ARG:HD2 | 4:B:1131:HOH:O | 2.18 | 0.43 |
| 1:J:700:MET:HE2 | 1:J:700:MET:HA | 2.01 | 0.43 |
| 1:B:684:LEU:CD2 | 1:B:688:MET:HG3 | 2.48 | 0.43 |
| 1:B:973:ILE:HG21 | 1:B:978:ASP:HB2 | 2.01 | 0.43 |
| 1:K:1003:TYR:HD2 | 1:K:1009:LEU:HG | 1.84 | 0.43 |
| 1:C:758:PRO:HD3 | 1:C:1011:GLY:H | 1.83 | 0.43 |
| 1:H:963:GLY:O | 1:H:973:ILE:HD12 | 2.19 | 0.43 |
| 1:K:748:ALA:HB3 | 1:K:936:ALA:HB1 | 2.01 | 0.43 |
| 1:J:959:PHE:CG | 1:J:977:MET:HE2 | 2.53 | 0.43 |
| 1:A:803:SER:HA | 1:A:811:LEU:HD11 | 2.01 | 0.43 |
| 1:F:716:PRO:HB2 | 1:F:719:GLN:HE22 | 1.84 | 0.43 |
| 1:J:716:PRO:HB2 | 1:J:719:GLN:HE22 | 1.83 | 0.43 |
| 1:L:845:ASN:O | 1:L:847:ARG:HG2 | 2.19 | 0.43 |
| 1:A:945:ARG:NH1 | 1:D:915:ASN:ND2 | 2.65 | 0.43 |
| 1:D:700:MET:CE | 1:D:746:LEU:HD21 | 2.49 | 0.43 |
| 1:E:915:ASN:O | 1:E:916:GLY:C | 2.58 | 0.43 |
| 1:D:705:GLN:HG2 | 1:D:710:LEU:HD12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:H:705:GLN:HG2 | 1:H:710:LEU:HD12 | 2.00 | 0.43 |
| 1:D:872:LEU:HD13 | 1:D:873:HIS:CD2 | 2.54 | 0.43 |
| 1:A:964:ASP:OD2 | 1:A:979:ARG:NH1 | 2.52 | 0.43 |
| 1:I:796:ASP:OD1 | 1:I:798:SER:CB | 2.67 | 0.43 |
| 1:H:905:PHE:CD1 | 1:H:931:VAL:HG21 | 2.54 | 0.43 |
| 1:K:957:ASN:O | 1:K:961:GLU:HG3 | 2.19 | 0.43 |
| 1:E:707:THR:HG21 | 1:E:709:LEU:HG | 2.00 | 0.42 |
| 1:F:705:GLN:HG2 | 1:F:710:LEU:HD12 | 2.02 | 0.42 |
| 1:A:794:ASN:HB3 | 1:A:799:TYR:HB2 | 2.00 | 0.42 |
| 1:E:758:PRO:HD3 | 1:E:1011:GLY:H | 1.84 | 0.42 |
| 1:E:964:ASP:OD2 | 1:E:979:ARG:NH1 | 2.52 | 0.42 |
| 1:J:758:PRO:HG3 | 1:J:799:TYR:HE2 | 1.84 | 0.42 |
| 1:K:737:HIS:CD2 | 1:K:958:GLU:OE2 | 2.59 | 0.42 |
| 1:F:845:ASN:O | 1:F:847:ARG:HG2 | 2.19 | 0.42 |
| 1:H:700:MET:HA | 1:H:700:MET:HE2 | 2.01 | 0.42 |
| 1:H:915:ASN:CG | 1:K:945:ARG:HH11 | 2.23 | 0.42 |
| 1:H:881:ARG:NH1 | 1:H:881:ARG:HG3 | 2.33 | 0.42 |
| 1:J:705:GLN:HG2 | 1:J:710:LEU:HD12 | 2.00 | 0.42 |
| 1:I:727:LEU:HD21 | 1:I:820:MET:HB3 | 2.02 | 0.42 |
| 1:G:803:SER:HA | 1:G:811:LEU:HD11 | 2.01 | 0.42 |
| 1:A:758:PRO:HD3 | 1:A:1011:GLY:H | 1.84 | 0.42 |
| 1:E:710:LEU:HD23 | 1:E:710:LEU:HA | 1.87 | 0.42 |
| 1:F:754:THR:HG22 | 1:F:755:ARG:NE | 2.34 | 0.42 |
| 1:D:952:THR:O | 1:D:956:VAL:HG22 | 2.19 | 0.42 |
| 1:D:700:MET:HE2 | 1:D:700:MET:HA | 2.00 | 0.42 |
| 1:C:883:ARG:HH12 | 1:D:846:ASP:CG | 2.21 | 0.42 |
| 1:B:1004:ASP:HA | 1:B:1009:LEU:HD12 | 2.00 | 0.42 |
| 1:I:917:ILE:O | 1:I:924:ASP:OD2 | 2.38 | 0.42 |
| 1:J:684:LEU:CD2 | 1:J:688:MET:HG3 | 2.49 | 0.42 |
| 1:I:677:TRP:NE1 | 1:I:943:LYS:HD3 | 2.34 | 0.42 |
| 1:D:851:GLU:HA | 1:D:854:HIS:HD2 | 1.83 | 0.42 |
| 1:C:957:ASN:O | 1:C:961:GLU:HG3 | 2.20 | 0.42 |
| 1:G:1014:LEU:N | 1:G:1056:ARG:O | 2.53 | 0.42 |
| 1:H:694:ARG:HA | 1:H:728:GLU:OE2 | 2.19 | 0.42 |
| 1:F:952:THR:O | 1:F:956:VAL:HG22 | 2.19 | 0.42 |
| 1:L:681:ILE:O | 1:L:685:VAL:HG23 | 2.19 | 0.42 |
| 1:B:721:MET:O | 1:B:725:ARG:HG2 | 2.20 | 0.42 |
| 1:I:684:LEU:HD23 | 1:I:684:LEU:O | 2.20 | 0.42 |
| 1:F:764:HIS:O | 1:F:766:GLY:N | 2.52 | 0.42 |
| 1:J:985:ALA:HA | 1:J:1072:TRP:HE3 | 1.84 | 0.42 |
| 1:J:663:LEU:HA | 1:J:666:GLU:OE1 | 2.19 | 0.42 |
| 1:B:796:ASP:OD1 | 1:B:798:SER:N | 2.41 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C:796:ASP:OD1 | 1:C:798:SER:CB | 2.68 | 0.42 |
| 1:J:703:LEU:HD22 | 1:J:750:TRP:CE2 | 2.54 | 0.42 |
| 1:F:1014:LEU:HD13 | 1:F:1056:ARG:HH21 | 1.84 | 0.42 |
| 1:J:956:VAL:HG23 | 1:J:957:ASN:N | 2.34 | 0.42 |
| 1:J:721:MET:O | 1:J:725:ARG:HG2 | 2.19 | 0.42 |
| 1:D:758:PRO:HG3 | 1:D:799:TYR:HE2 | 1.84 | 0.42 |
| 1:L:755:ARG:HD2 | 4:L:1631:HOH:O | 2.20 | 0.42 |
| 1:J:694:ARG:HA | 1:J:728:GLU:OE2 | 2.19 | 0.42 |
| 1:J:952:THR:O | 1:J:956:VAL:HG22 | 2.20 | 0.42 |
| 1:H:915:ASN:ND2 | 1:K:945:ARG:HH11 | 2.18 | 0.42 |
| 1:A:871:LEU:HB3 | 1:A:874:LEU:HD12 | 2.01 | 0.42 |
| 1:F:915:ASN:CG | 1:I:945:ARG:NH1 | 2.73 | 0.42 |
| 1:L:703:LEU:HD22 | 1:L:750:TRP:CE2 | 2.54 | 0.42 |
| 1:L:663:LEU:HA | 1:L:666:GLU:OE1 | 2.20 | 0.42 |
| 1:L:851:GLU:HA | 1:L:854:HIS:HD2 | 1.85 | 0.42 |
| 1:L:716:PRO:HB2 | 1:L:719:GLN:HE22 | 1.85 | 0.42 |
| 1:G:737:HIS:CD2 | 1:G:958:GLU:OE2 | 2.60 | 0.42 |
| 1:F:725:ARG:HG3 | 1:F:725:ARG:NH1 | 2.33 | 0.42 |
| 1:H:710:LEU:HD23 | 1:H:715:ILE:HB | 2.02 | 0.42 |
| 1:H:938:ILE:HD12 | 1:H:996:VAL:HG22 | 2.01 | 0.42 |
| 1:E:969:LEU:HD23 | 1:H:873:HIS:CD2 | 2.54 | 0.42 |
| 1:G:862:TYR:OH | 1:G:869:ASN:ND2 | 2.52 | 0.42 |
| 1:H:973:ILE:HG21 | 1:H:978:ASP:HB2 | 2.00 | 0.42 |
| 1:B:905:PHE:CD1 | 1:B:931:VAL:HG21 | 2.54 | 0.42 |
| 1:B:663:LEU:HA | 1:B:666:GLU:OE1 | 2.19 | 0.42 |
| 1:I:991:PHE:CD1 | 1:I:995:ILE:HD12 | 2.54 | 0.42 |
| 1:G:814:LEU:HD11 | 1:G:933:ILE:HB | 2.01 | 0.42 |
| 1:A:934:LYS:HB3 | 1:A:934:LYS:HZ2 | 1.85 | 0.42 |
| 1:A:842:VAL:HA | 1:B:883:ARG:HH22 | 1.84 | 0.42 |
| 1:C:803:SER:HA | 1:C:811:LEU:HD11 | 2.02 | 0.42 |
| 1:C:814:LEU:HD11 | 1:C:933:ILE:HB | 2.02 | 0.42 |
| 1:D:980:SER:O | 1:D:981:SER:HB2 | 2.19 | 0.42 |
| 1:I:969:LEU:HD23 | 1:L:873:HIS:HD2 | 1.82 | 0.42 |
| 1:D:710:LEU:HD23 | 1:D:715:ILE:HB | 2.02 | 0.42 |
| 1:L:1059:CYS:HB3 | 1:L:1062:MET:CB | 2.49 | 0.42 |
| 1:A:939:ASN:O | 1:A:940:GLY:C | 2.58 | 0.42 |
| 1:G:869:ASN:ND2 | 1:G:869:ASN:C | 2.73 | 0.42 |
| 1:A:872:LEU:HD12 | 1:A:873:HIS:H | 1.85 | 0.42 |
| 1:J:723:TYR:CE1 | 1:J:861:LEU:HD13 | 2.55 | 0.42 |
| 1:D:880:LYS:HA | 1:D:880:LYS:HD2 | 1.88 | 0.42 |
| 1:G:934:LYS:HZ2 | 1:G:934:LYS:HB3 | 1.85 | 0.42 |
| 1:G:962:GLN:O | 1:G:966:GLU:HG3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:H:695:ILE:HG22 | 1:H:743:THR:HG21 | 2.01 | 0.42 |
| 1:L:700:MET:HE3 | 1:L:746:LEU:HD13 | 2.02 | 0.42 |
| 1:L:881:ARG:NH1 | 1:L:881:ARG:HG3 | 2.34 | 0.42 |
| 1:A:674:MET:HE1 | 1:A:703:LEU:HD21 | 2.02 | 0.42 |
| 1:J:930:GLN:O | 1:J:933:ILE:HG13 | 2.20 | 0.42 |
| 1:D:663:LEU:HA | 1:D:666:GLU:OE1 | 2.20 | 0.42 |
| 1:K:872:LEU:HD12 | 1:K:873:HIS:H | 1.85 | 0.42 |
| 1:C:915:ASN:O | 1:C:916:GLY:C | 2.58 | 0.42 |
| 1:B:763:ILE:O | 1:B:764:HIS:CB | 2.67 | 0.42 |
| 1:J:1004:ASP:HA | 1:J:1009:LEU:HD12 | 2.01 | 0.42 |
| 1:E:914:SER:OG | 1:E:915:ASN:N | 2.52 | 0.42 |
| 1:L:1003:TYR:HD2 | 1:L:1009:LEU:HG | 1.83 | 0.42 |
| 1:E:872:LEU:HD13 | 1:E:873:HIS:CD2 | 2.54 | 0.42 |
| 1:K:1004:ASP:HB2 | 1:K:1009:LEU:HD12 | 2.02 | 0.42 |
| 1:K:872:LEU:HD13 | 1:K:873:HIS:CG | 2.54 | 0.42 |
| 1:E:944:VAL:HG22 | 1:E:945:ARG:N | 2.35 | 0.42 |
| 1:B:758:PRO:HG3 | 1:B:799:TYR:HE2 | 1.85 | 0.42 |
| 1:F:974:SER:HB2 | 1:F:977:MET:SD | 2.59 | 0.42 |
| 1:G:784:ILE:HG21 | 1:G:807:PRO:HB3 | 2.00 | 0.42 |
| 1:B:952:THR:O | 1:B:956:VAL:HG22 | 2.20 | 0.41 |
| 1:L:754:THR:HG22 | 1:L:755:ARG:NE | 2.35 | 0.41 |
| 1:G:707:THR:HG21 | 1:G:709:LEU:HG | 2.01 | 0.41 |
| 1:A:952:THR:O | 1:A:956:VAL:HG22 | 2.20 | 0.41 |
| 1:C:727:LEU:HD21 | 1:C:820:MET:HB3 | 2.02 | 0.41 |
| 1:J:963:GLY:O | 1:J:973:ILE:HD12 | 2.19 | 0.41 |
| 1:C:915:ASN:HD22 | 1:C:915:ASN:HA | 1.63 | 0.41 |
| 1:C:694:ARG:O | 1:C:698:GLN:HG2 | 2.20 | 0.41 |
| 1:D:974:SER:HB2 | 1:D:977:MET:SD | 2.60 | 0.41 |
| 1:C:976:PHE:CG | 1:C:987:LEU:HD13 | 2.55 | 0.41 |
| 1:K:796:ASP:OD1 | 1:K:798:SER:CB | 2.68 | 0.41 |
| 1:C:825:HIS:CD2 | 1:C:826:PRO:HD2 | 2.55 | 0.41 |
| 1:L:980:SER:O | 1:L:981:SER:HB2 | 2.20 | 0.41 |
| 1:L:1004:ASP:HA | 1:L:1009:LEU:HD12 | 2.01 | 0.41 |
| 1:H:700:MET:CE | 1:H:746:LEU:CD2 | 2.98 | 0.41 |
| 1:J:710:LEU:HD23 | 1:J:715:ILE:HB | 2.03 | 0.41 |
| 1:D:963:GLY:O | 1:D:973:ILE:HD12 | 2.20 | 0.41 |
| 1:D:991:PHE:CE2 | 1:D:996:VAL:HG23 | 2.54 | 0.41 |
| 1:H:959:PHE:CB | 1:H:977:MET:HE2 | 2.51 | 0.41 |
| 1:A:846:ASP:OD2 | 1:B:883:ARG:NH1 | 2.53 | 0.41 |
| 1:E:670:LEU:HD22 | 1:E:674:MET:SD | 2.60 | 0.41 |
| 1:I:1068:ASN:O | 1:I:1071:ILE:HG12 | 2.20 | 0.41 |
| 1:A:891:LEU:HD13 | 1:B:847:ARG:NH2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:H:755:ARG:HA | 1:H:756:PRO:HD3 | 1.91 | 0.41 |
| 1:B:751:TYR:CE1 | 1:B:755:ARG:HG3 | 2.55 | 0.41 |
| 1:L:694:ARG:HA | 1:L:728:GLU:OE2 | 2.20 | 0.41 |
| 1:H:670:LEU:HD22 | 1:H:674:MET:SD | 2.60 | 0.41 |
| 1:G:952:THR:O | 1:G:956:VAL:HG22 | 2.20 | 0.41 |
| 1:F:963:GLY:O | 1:F:973:ILE:HD12 | 2.20 | 0.41 |
| 1:K:988:GLN:HA | 1:K:988:GLN:OE1 | 2.21 | 0.41 |
| 1:I:939:ASN:O | 1:I:940:GLY:C | 2.58 | 0.41 |
| 1:B:713:PHE:O | 1:B:714:LYS:C | 2.58 | 0.41 |
| 1:F:703:LEU:HD22 | 1:F:750:TRP:CE2 | 2.55 | 0.41 |
| 1:D:905:PHE:CD1 | 1:D:931:VAL:HG21 | 2.55 | 0.41 |
| 1:L:751:TYR:CE2 | 1:L:755:ARG:HG3 | 2.55 | 0.41 |
| 1:L:700:MET:CE | 1:L:746:LEU:CD2 | 2.99 | 0.41 |
| 1:I:915:ASN:O | 1:I:916:GLY:C | 2.58 | 0.41 |
| 1:C:674:MET:CE | 1:C:703:LEU:HD21 | 2.50 | 0.41 |
| 1:H:663:LEU:HA | 1:H:666:GLU:OE1 | 2.19 | 0.41 |
| 1:K:1068:ASN:O | 1:K:1071:ILE:HG12 | 2.20 | 0.41 |
| 1:D:1059:CYS:HB3 | 1:D:1062:MET:CB | 2.51 | 0.41 |
| 1:H:703:LEU:HD22 | 1:H:750:TRP:CE2 | 2.54 | 0.41 |
| 1:G:853:HIS:O | 1:G:857:SER:HB2 | 2.21 | 0.41 |
| 1:B:751:TYR:CE2 | 1:B:755:ARG:HG3 | 2.55 | 0.41 |
| 1:B:812:MET:O | 1:B:816:VAL:HG23 | 2.20 | 0.41 |
| 1:G:915:ASN:O | 1:G:916:GLY:C | 2.58 | 0.41 |
| 1:A:717:THR:OG1 | 1:J:1019:ASP:HA | 2.20 | 0.41 |
| 1:G:762:GLN:CD | 1:G:800:GLY:HA2 | 2.41 | 0.41 |
| 1:A:796:ASP:OD1 | 1:A:798:SER:CB | 2.69 | 0.41 |
| 1:H:796:ASP:OD1 | 1:H:798:SER:N | 2.41 | 0.41 |
| 1:E:736:TYR:CD1 | 1:E:955:ILE:HG13 | 2.55 | 0.41 |
| 1:L:723:TYR:CE1 | 1:L:861:LEU:HD13 | 2.56 | 0.41 |
| 1:I:710:LEU:HA | 1:I:710:LEU:HD23 | 1.87 | 0.41 |
| 1:C:1003:TYR:HD2 | 1:C:1009:LEU:HG | 1.85 | 0.41 |
| 1:H:980:SER:O | 1:H:981:SER:HB2 | 2.19 | 0.41 |
| 1:A:902:LEU:HA | 1:A:902:LEU:HD12 | 1.93 | 0.41 |
| 1:F:1003:TYR:HD2 | 1:F:1009:LEU:HG | 1.82 | 0.41 |
| 1:G:1071:ILE:HG21 | 1:L:915:ASN:ND2 | 2.36 | 0.41 |
| 1:F:881:ARG:NH1 | 1:F:881:ARG:HG3 | 2.35 | 0.41 |
| 1:B:938:ILE:HD12 | 1:B:996:VAL:HG22 | 2.02 | 0.41 |
| 1:E:872:LEU:HD12 | 1:E:873:HIS:H | 1.83 | 0.41 |
| 1:I:814:LEU:HD11 | 1:I:933:ILE:HB | 2.02 | 0.41 |
| 1:B:723:TYR:CE1 | 1:B:861:LEU:HD13 | 2.56 | 0.41 |
| 1:B:930:GLN:O | 1:B:933:ILE:HG13 | 2.20 | 0.41 |
| 1:G:681:ILE:HG23 | 1:G:682:PHE:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:L:880:LYS:HD2 | 1:L:880:LYS:HA | 1.87 | 0.41 |
| 1:K:762:GLN:NE2 | 1:K:804:SER:CB | 2.78 | 0.41 |
| 1:H:751:TYR:CE1 | 1:H:755:ARG:HG3 | 2.55 | 0.41 |
| 1:D:721:MET:O | 1:D:725:ARG:HG2 | 2.19 | 0.41 |
| 1:I:674:MET:CE | 1:I:703:LEU:HD21 | 2.50 | 0.41 |
| 1:B:959:PHE:CG | 1:B:977:MET:HE2 | 2.56 | 0.41 |
| 1:E:953:GLU:O | 1:E:957:ASN:ND2 | 2.54 | 0.41 |
| 1:G:763:ILE:C | 1:G:765:ASN:H | 2.23 | 0.41 |
| 1:I:784:ILE:HG21 | 1:I:807:PRO:HB3 | 2.02 | 0.41 |
| 1:F:663:LEU:HA | 1:F:666:GLU:OE1 | 2.21 | 0.41 |
| 1:A:844:TYR:CE2 | 1:A:852:ASN:HB3 | 2.55 | 0.41 |
| 1:D:716:PRO:HB2 | 1:D:719:GLN:NE2 | 2.35 | 0.41 |
| 1:J:754:THR:HG22 | 1:J:755:ARG:NE | 2.34 | 0.41 |
| 1:C:917:ILE:O | 1:C:924:ASP:OD2 | 2.38 | 0.41 |
| 1:G:944:VAL:HG22 | 1:G:945:ARG:N | 2.36 | 0.41 |
| 1:C:713:PHE:O | 1:C:714:LYS:C | 2.57 | 0.41 |
| 1:F:670:LEU:O | 1:F:674:MET:HG3 | 2.20 | 0.41 |
| 1:I:939:ASN:ND2 | 1:I:943:LYS:HE3 | 2.36 | 0.41 |
| 1:D:959:PHE:CG | 1:D:977:MET:HE2 | 2.56 | 0.41 |
| 1:I:952:THR:HG23 | 1:I:988:GLN:NE2 | 2.35 | 0.41 |
| 1:C:762:GLN:HA | 1:C:805:ASN:HD21 | 1.86 | 0.41 |
| 1:I:1003:TYR:HD2 | 1:I:1009:LEU:HG | 1.86 | 0.41 |
| 1:L:943:LYS:HG3 | 1:L:943:LYS:HZ2 | 1.76 | 0.41 |
| 1:D:1014:LEU:HD21 | 1:D:1058:PHE:HB2 | 2.03 | 0.41 |
| 1:B:754:THR:HG22 | 1:B:755:ARG:NE | 2.35 | 0.41 |
| 1:B:980:SER:O | 1:B:981:SER:HB2 | 2.20 | 0.41 |
| 1:L:700:MET:HE3 | 1:L:746:LEU:CD1 | 2.50 | 0.41 |
| 1:F:685:VAL:HG22 | 1:F:695:ILE:HD11 | 2.03 | 0.41 |
| 1:F:1004:ASP:HA | 1:F:1009:LEU:HD12 | 2.02 | 0.41 |
| 1:K:917:ILE:O | 1:K:924:ASP:OD2 | 2.38 | 0.41 |
| 1:B:885:LEU:HA | 1:B:885:LEU:HD12 | 1.79 | 0.41 |
| 1:J:881:ARG:HG3 | 1:J:881:ARG:NH1 | 2.35 | 0.41 |
| 1:G:871:LEU:HB3 | 1:G:874:LEU:HD12 | 2.02 | 0.41 |
| 1:L:967:ALA:HB2 | 1:L:973:ILE:HD11 | 2.03 | 0.41 |
| 1:I:872:LEU:HD12 | 1:I:873:HIS:H | 1.85 | 0.41 |
| 1:I:991:PHE:CE2 | 1:I:996:VAL:HG23 | 2.56 | 0.41 |
| 1:C:976:PHE:CD2 | 1:C:987:LEU:HB2 | 2.56 | 0.41 |
| 1:B:681:ILE:H | 1:B:681:ILE:HG13 | 1.46 | 0.41 |
| 1:G:872:LEU:HD13 | 1:G:873:HIS:CG | 2.56 | 0.41 |
| 1:E:715:ILE:HA | 1:E:716:PRO:HD2 | 1.96 | 0.41 |
| 1:H:758:PRO:HG3 | 1:H:799:TYR:HE2 | 1.85 | 0.41 |
| 1:C:979:ARG:O | 1:C:982:PRO:HD3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:748:ALA:HB3 | 1:A:936:ALA:HB1 | 2.03 | 0.41 |
| 1:E:694:ARG:O | 1:E:698:GLN:HG2 | 2.21 | 0.41 |
| 1:E:976:PHE:CG | 1:E:987:LEU:HD13 | 2.56 | 0.41 |
| 1:D:1015:GLU:HG3 | 1:D:1015:GLU:H | 1.76 | 0.41 |
| 1:E:803:SER:HA | 1:E:811:LEU:HD11 | 2.02 | 0.41 |
| 1:B:828:ARG:NH2 | 4:B:1129:HOH:O | 2.54 | 0.41 |
| 1:B:881:ARG:HG2 | 1:B:885:LEU:HD22 | 2.02 | 0.41 |
| 1:E:871:LEU:HB3 | 1:E:874:LEU:HD12 | 2.03 | 0.41 |
| 1:L:710:LEU:HD23 | 1:L:715:ILE:HB | 2.03 | 0.41 |
| 1:G:713:PHE:O | 1:G:714:LYS:C | 2.58 | 0.41 |
| 1:C:952:THR:HG23 | 1:C:988:GLN:NE2 | 2.36 | 0.41 |
| 1:C:795:PRO:HD2 | 1:C:799:TYR:CD1 | 2.56 | 0.41 |
| 1:K:953:GLU:O | 1:K:957:ASN:ND2 | 2.54 | 0.41 |
| 1:K:704:PHE:HB3 | 1:K:710:LEU:HG | 2.03 | 0.41 |
| 1:J:900:ASP:OD1 | 1:J:900:ASP:N | 2.54 | 0.41 |
| 1:B:825:HIS:CD2 | 1:B:826:PRO:HD2 | 2.56 | 0.40 |
| 1:A:913:ASN:HA | 1:C:1056:ARG:HE | 1.85 | 0.40 |
| 1:A:915:ASN:O | 1:A:916:GLY:C | 2.59 | 0.40 |
| 1:D:1003:TYR:HD2 | 1:D:1009:LEU:HG | 1.85 | 0.40 |
| 1:F:881:ARG:HG2 | 1:F:885:LEU:HD22 | 2.03 | 0.40 |
| 1:J:805:ASN:HD22 | 1:J:805:ASN:N | 2.19 | 0.40 |
| 1:J:1015:GLU:OE1 | 1:J:1019:ASP:HB2 | 2.20 | 0.40 |
| 1:C:872:LEU:HD13 | 1:C:873:HIS:CD2 | 2.57 | 0.40 |
| 1:C:872:LEU:HD13 | 1:C:873:HIS:CG | 2.56 | 0.40 |
| 1:E:814:LEU:HD11 | 1:E:933:ILE:HB | 2.02 | 0.40 |
| 1:J:905:PHE:CD1 | 1:J:931:VAL:HG21 | 2.56 | 0.40 |
| 1:J:885:LEU:HA | 1:J:885:LEU:HD12 | 1.81 | 0.40 |
| 1:K:853:HIS:O | 1:K:857:SER:HB2 | 2.22 | 0.40 |
| 1:D:751:TYR:CE2 | 1:D:755:ARG:HG3 | 2.56 | 0.40 |
| 1:J:751:TYR:CE2 | 1:J:755:ARG:HG3 | 2.56 | 0.40 |
| 1:L:952:THR:O | 1:L:956:VAL:HG22 | 2.20 | 0.40 |
| 1:F:956:VAL:HG23 | 1:F:957:ASN:N | 2.36 | 0.40 |
| 1:D:694:ARG:HA | 1:D:728:GLU:OE2 | 2.21 | 0.40 |
| 1:A:711:GLU:OE2 | 1:J:1013:TRP:HB2 | 2.21 | 0.40 |
| 1:J:674:MET:HE3 | 1:J:699:VAL:HG13 | 2.03 | 0.40 |
| 1:A:962:GLN:O | 1:A:966:GLU:HG3 | 2.22 | 0.40 |
| 1:I:758:PRO:HD3 | 1:I:1011:GLY:H | 1.86 | 0.40 |
| 1:C:1015:GLU:HB3 | 1:C:1016:ALA:H | 1.77 | 0.40 |
| 1:K:758:PRO:HD3 | 1:K:1011:GLY:H | 1.85 | 0.40 |
| 1:H:880:LYS:HA | 1:H:880:LYS:HD2 | 1.86 | 0.40 |
| 1:L:948:HIS:CD2 | 1:L:1068:ASN:HB3 | 2.56 | 0.40 |
| 1:J:1068:ASN:O | 1:J:1071:ILE:HG12 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:I:700:MET:HE3 | 1:I:746:LEU:CD1 | 2.51 | 0.40 |
| 1:F:980:SER:O | 1:F:981:SER:HB2 | 2.21 | 0.40 |
| 1:E:1071:ILE:HG22 | 1:J:915:ASN:HD22 | 1.85 | 0.40 |
| 1:I:802:LEU:HD22 | 1:I:802:LEU:N | 2.36 | 0.40 |
| 1:J:980:SER:O | 1:J:981:SER:HB2 | 2.21 | 0.40 |
| 1:D:1069:HIS:CE1 | 1:D:1073:LYS:NZ | 2.89 | 0.40 |
| 1:K:939:ASN:O | 1:K:940:GLY:C | 2.60 | 0.40 |
| 1:C:748:ALA:HB3 | 1:C:936:ALA:HB1 | 2.03 | 0.40 |
| 1:I:694:ARG:O | 1:I:698:GLN:HG2 | 2.21 | 0.40 |
| 1:C:1068:ASN:O | 1:C:1071:ILE:HG12 | 2.21 | 0.40 |
| 1:H:716:PRO:HB2 | 1:H:719:GLN:NE2 | 2.36 | 0.40 |
| 1:K:754:THR:HG22 | 1:K:755:ARG:NE | 2.22 | 0.40 |
| 1:H:754:THR:HG22 | 1:H:755:ARG:NE | 2.35 | 0.40 |
| 1:H:681:ILE:O | 1:H:685:VAL:HG23 | 2.21 | 0.40 |
| 1:A:944:VAL:HG22 | 1:A:945:ARG:N | 2.37 | 0.40 |
| 1:B:1069:HIS:CE1 | 1:B:1073:LYS:NZ | 2.90 | 0.40 |
| 1:C:881:ARG:HG3 | 1:C:881:ARG:NH1 | 2.35 | 0.40 |
| 1:H:670:LEU:O | 1:H:674:MET:HG3 | 2.21 | 0.40 |
| 1:H:674:MET:HE3 | 1:H:699:VAL:HG13 | 2.03 | 0.40 |
| 1:A:930:GLN:O | 1:A:934:LYS:HG3 | 2.22 | 0.40 |
| 1:D:1059:CYS:HB3 | 1:D:1062:MET:HB2 | 2.03 | 0.40 |
| 1:H:1019:ASP:OD2 | 1:H:1055:ARG:HA | 2.21 | 0.40 |
| 1:K:905:PHE:CD1 | 1:K:931:VAL:HG21 | 2.56 | 0.40 |
| 1:K:814:LEU:HD11 | 1:K:933:ILE:HB | 2.02 | 0.40 |
| 1:L:900:ASP:N | 1:L:900:ASP:OD1 | 2.55 | 0.40 |
| 1:B:900:ASP:OD1 | 1:B:900:ASP:N | 2.55 | 0.40 |
| 1:G:754:THR:CG2 | 1:G:755:ARG:HE | 2.22 | 0.40 |
| 1:K:735:PRO:HG2 | 1:K:958:GLU:HB2 | 2.03 | 0.40 |
| 1:E:743:THR:O | 1:E:746:LEU:HB3 | 2.22 | 0.40 |
| 1:H:1004:ASP:CA | 1:H:1009:LEU:HD12 | 2.51 | 0.40 |
| 1:E:712:ILE:H | 1:E:712:ILE:HG13 | 1.77 | 0.40 |
| 1:D:967:ALA:HB2 | 1:D:973:ILE:HD11 | 2.04 | 0.40 |
| 1:C:939:ASN:O | 1:C:940:GLY:C | 2.60 | 0.40 |
| 1:E:951:TRP:O | 1:E:955:ILE:HD12 | 2.22 | 0.40 |
| 1:C:1004:ASP:CB | 1:C:1009:LEU:HD12 | 2.52 | 0.40 |
| 1:B:1059:CYS:HB3 | 1:B:1062:MET:HB2 | 2.03 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 358/420 (85%) | 332 (93%) | 21 (6%) | 5 (1%) | 16 | 52 |
| 1 | B | 375/420 (89%) | 337 (90%) | 28 (8%) | 10 (3%) | 8 | 30 |
| 1 | C | 358/420 (85%) | 330 (92%) | 22 (6%) | 6 (2%) | 14 | 45 |
| 1 | D | 375/420 (89%) | 334 (89%) | 31 (8%) | 10 (3%) | 8 | 30 |
| 1 | E | 358/420 (85%) | 334 (93%) | 18 (5%) | 6 (2%) | 14 | 45 |
| 1 | F | 375/420 (89%) | 335 (89%) | 31 (8%) | 9 (2%) | 9 | 35 |
| 1 | G | 358/420 (85%) | 333 (93%) | 22 (6%) | 3 (1%) | 27 | 68 |
| 1 | H | 375/420 (89%) | 339 (90%) | 28 (8%) | 8 (2%) | 11 | 39 |
| 1 | I | 358/420 (85%) | 332 (93%) | 20 (6%) | 6 (2%) | 14 | 45 |
| 1 | J | 375/420 (89%) | 338 (90%) | 28 (8%) | 9 (2%) | 9 | 35 |
| 1 | K | 358/420 (85%) | 327 (91%) | 25 (7%) | 6 (2%) | 14 | 45 |
| 1 | L | 375/420 (89%) | 334 (89%) | 30 (8%) | 11 (3%) | 7 | 28 |
| All | All | 4398/5040 (87%) | 4005 (91%) | 304 (7%) | 89 (2%) | 11 | 40 |

All (89) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 869 | ASN |
| 1 | C | 765 | ASN |
| 1 | C | 869 | ASN |
| 1 | D | 764 | HIS |
| 1 | E | 763 | ILE |
| 1 | E | 869 | ASN |
| 1 | F | 764 | HIS |
| 1 | F | 765 | ASN |
| 1 | H | 764 | HIS |
| 1 | I | 763 | ILE |
| 1 | I | 765 | ASN |
| 1 | I | 869 | ASN |
| 1 | J | 764 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | K | 763 | ILE |
| 1 | K | 765 | ASN |
| 1 | K | 869 | ASN |
| 1 | L | 764 | HIS |
| 1 | A | 916 | GLY |
| 1 | B | 764 | HIS |
| 1 | B | 1071 | ILE |
| 1 | C | 916 | GLY |
| 1 | D | 763 | ILE |
| 1 | D | 765 | ASN |
| 1 | D | 1054 | ARG |
| 1 | D | 1071 | ILE |
| 1 | E | 765 | ASN |
| 1 | E | 916 | GLY |
| 1 | F | 1054 | ARG |
| 1 | F | 1071 | ILE |
| 1 | G | 869 | ASN |
| 1 | G | 916 | GLY |
| 1 | H | 1071 | ILE |
| 1 | I | 916 | GLY |
| 1 | J | 763 | ILE |
| 1 | J | 1023 | GLU |
| 1 | J | 1071 | ILE |
| 1 | K | 916 | GLY |
| 1 | L | 1020 | ASN |
| 1 | L | 1071 | ILE |
| 1 | A | 765 | ASN |
| 1 | B | 675 | SER |
| 1 | C | 764 | HIS |
| 1 | J | 675 | SER |
| 1 | J | 765 | ASN |
| 1 | L | 763 | ILE |
| 1 | L | 765 | ASN |
| 1 | L | 869 | ASN |
| 1 | A | 940 | GLY |
| 1 | B | 869 | ASN |
| 1 | B | 940 | GLY |
| 1 | B | 981 | SER |
| 1 | D | 869 | ASN |
| 1 | D | 981 | SER |
| 1 | E | 940 | GLY |
| 1 | F | 675 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | F | 869 | ASN |
| 1 | F | 981 | SER |
| 1 | H | 675 | SER |
| 1 | H | 869 | ASN |
| 1 | H | 981 | SER |
| 1 | J | 869 | ASN |
| 1 | J | 981 | SER |
| 1 | K | 940 | GLY |
| 1 | L | 675 | SER |
| 1 | L | 940 | GLY |
| 1 | L | 981 | SER |
| 1 | L | 1023 | GLU |
| 1 | B | 763 | ILE |
| 1 | B | 765 | ASN |
| 1 | C | 940 | GLY |
| 1 | D | 675 | SER |
| 1 | D | 940 | GLY |
| 1 | F | 763 | ILE |
| 1 | H | 940 | GLY |
| 1 | I | 940 | GLY |
| 1 | B | 1017 | GLU |
| 1 | G | 940 | GLY |
| 1 | H | 1054 | ARG |
| 1 | J | 940 | GLY |
| 1 | F | 940 | GLY |
| 1 | E | 849 | VAL |
| 1 | I | 849 | VAL |
| 1 | K | 849 | VAL |
| 1 | B | 941 | PRO |
| 1 | C | 849 | VAL |
| 1 | L | 941 | PRO |
| 1 | A | 849 | VAL |
| 1 | D | 941 | PRO |
| 1 | H | 941 | PRO |

5.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 306/370 (83%) | 288 (94%) | 18 (6%) | 28 | 64 |
| 1 | B | 313/370 (85%) | 291 (93%) | 22 (7%) | 21 | 53 |
| 1 | C | 306/370 (83%) | 290 (95%) | 16 (5%) | 32 | 71 |
| 1 | D | 313/370 (85%) | 291 (93%) | 22 (7%) | 21 | 53 |
| 1 | E | 306/370 (83%) | 291 (95%) | 15 (5%) | 35 | 73 |
| 1 | F | 313/370 (85%) | 292 (93%) | 21 (7%) | 23 | 56 |
| 1 | G | 306/370 (83%) | 287 (94%) | 19 (6%) | 26 | 61 |
| 1 | H | 313/370 (85%) | 291 (93%) | 22 (7%) | 21 | 53 |
| 1 | I | 306/370 (83%) | 288 (94%) | 18 (6%) | 28 | 64 |
| 1 | J | 313/370 (85%) | 292 (93%) | 21 (7%) | 23 | 56 |
| 1 | K | 306/370 (83%) | 288 (94%) | 18 (6%) | 28 | 64 |
| 1 | L | 313/370 (85%) | 292 (93%) | 21 (7%) | 23 | 56 |
| All | All | 3714/4440 (84%) | 3481 (94%) | 233 (6%) | 25 | 60 |

All (233) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 670 | LEU |
| 1 | A | 684 | LEU |
| 1 | A | 686 | GLU |
| 1 | A | 694 | ARG |
| 1 | A | 706 | ASP |
| 1 | A | 719 | GLN |
| 1 | A | 755 | ARG |
| 1 | A | 792 | CYS |
| 1 | A | 828 | ARG |
| 1 | A | 857 | SER |
| 1 | A | 861 | LEU |
| 1 | A | 869 | ASN |
| 1 | A | 872 | LEU |
| 1 | A | 885 | LEU |
| 1 | A | 915 | ASN |
| 1 | A | 924 | ASP |
| 1 | A | 965 | GLU |
| 1 | A | 1061 | LEU |
| 1 | B | 670 | LEU |
| 1 | B | 681 | ILE |
| 1 | B | 692 | SER |
| 1 | B | 719 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 739 | ARG |
| 1 | B | 792 | CYS |
| 1 | B | 802 | LEU |
| 1 | B | 828 | ARG |
| 1 | B | 847 | ARG |
| 1 | B | 857 | SER |
| 1 | B | 861 | LEU |
| 1 | B | 872 | LEU |
| 1 | B | 885 | LEU |
| 1 | B | 900 | ASP |
| 1 | B | 910 | ASN |
| 1 | B | 911 | ASP |
| 1 | B | 933 | ILE |
| 1 | B | 935 | LEU |
| 1 | B | 947 | LEU |
| 1 | B | 1015 | GLU |
| 1 | B | 1019 | ASP |
| 1 | B | 1057 | ILE |
| 1 | C | 670 | LEU |
| 1 | C | 684 | LEU |
| 1 | C | 686 | GLU |
| 1 | C | 694 | ARG |
| 1 | C | 706 | ASP |
| 1 | C | 719 | GLN |
| 1 | C | 755 | ARG |
| 1 | C | 792 | CYS |
| 1 | C | 828 | ARG |
| 1 | C | 857 | SER |
| 1 | C | 861 | LEU |
| 1 | C | 869 | ASN |
| 1 | C | 872 | LEU |
| 1 | C | 915 | ASN |
| 1 | C | 965 | GLU |
| 1 | C | 1061 | LEU |
| 1 | D | 670 | LEU |
| 1 | D | 681 | ILE |
| 1 | D | 692 | SER |
| 1 | D | 719 | GLN |
| 1 | D | 739 | ARG |
| 1 | D | 792 | CYS |
| 1 | D | 802 | LEU |
| 1 | D | 828 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 847 | ARG |
| 1 | D | 857 | SER |
| 1 | D | 861 | LEU |
| 1 | D | 872 | LEU |
| 1 | D | 885 | LEU |
| 1 | D | 900 | ASP |
| 1 | D | 910 | ASN |
| 1 | D | 911 | ASP |
| 1 | D | 933 | ILE |
| 1 | D | 935 | LEU |
| 1 | D | 947 | LEU |
| 1 | D | 1015 | GLU |
| 1 | D | 1020 | ASN |
| 1 | D | 1057 | ILE |
| 1 | E | 670 | LEU |
| 1 | E | 684 | LEU |
| 1 | E | 686 | GLU |
| 1 | E | 694 | ARG |
| 1 | E | 706 | ASP |
| 1 | E | 719 | GLN |
| 1 | E | 792 | CYS |
| 1 | E | 828 | ARG |
| 1 | E | 857 | SER |
| 1 | E | 861 | LEU |
| 1 | E | 869 | ASN |
| 1 | E | 872 | LEU |
| 1 | E | 915 | ASN |
| 1 | E | 965 | GLU |
| 1 | E | 1061 | LEU |
| 1 | F | 670 | LEU |
| 1 | F | 681 | ILE |
| 1 | F | 692 | SER |
| 1 | F | 719 | GLN |
| 1 | F | 739 | ARG |
| 1 | F | 802 | LEU |
| 1 | F | 828 | ARG |
| 1 | F | 847 | ARG |
| 1 | F | 857 | SER |
| 1 | F | 861 | LEU |
| 1 | F | 872 | LEU |
| 1 | F | 885 | LEU |
| 1 | F | 900 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | F | 910 | ASN |
| 1 | F | 911 | ASP |
| 1 | F | 933 | ILE |
| 1 | F | 935 | LEU |
| 1 | F | 947 | LEU |
| 1 | F | 1015 | GLU |
| 1 | F | 1057 | ILE |
| 1 | F | 1059 | CYS |
| 1 | G | 670 | LEU |
| 1 | G | 684 | LEU |
| 1 | G | 686 | GLU |
| 1 | G | 694 | ARG |
| 1 | G | 706 | ASP |
| 1 | G | 719 | GLN |
| 1 | G | 755 | ARG |
| 1 | G | 792 | CYS |
| 1 | G | 828 | ARG |
| 1 | G | 857 | SER |
| 1 | G | 861 | LEU |
| 1 | G | 869 | ASN |
| 1 | G | 872 | LEU |
| 1 | G | 885 | LEU |
| 1 | G | 915 | ASN |
| 1 | G | 924 | ASP |
| 1 | G | 965 | GLU |
| 1 | G | 1000 | CYS |
| 1 | G | 1061 | LEU |
| 1 | H | 670 | LEU |
| 1 | H | 681 | ILE |
| 1 | H | 692 | SER |
| 1 | H | 719 | GLN |
| 1 | H | 739 | ARG |
| 1 | H | 776 | ASP |
| 1 | H | 802 | LEU |
| 1 | H | 828 | ARG |
| 1 | H | 847 | ARG |
| 1 | H | 857 | SER |
| 1 | H | 861 | LEU |
| 1 | H | 872 | LEU |
| 1 | H | 885 | LEU |
| 1 | H | 900 | ASP |
| 1 | H | 910 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | H | 911 | ASP |
| 1 | H | 933 | ILE |
| 1 | H | 935 | LEU |
| 1 | H | 947 | LEU |
| 1 | H | 1015 | GLU |
| 1 | H | 1056 | ARG |
| 1 | H | 1057 | ILE |
| 1 | I | 670 | LEU |
| 1 | I | 684 | LEU |
| 1 | I | 686 | GLU |
| 1 | I | 694 | ARG |
| 1 | I | 706 | ASP |
| 1 | I | 719 | GLN |
| 1 | I | 755 | ARG |
| 1 | I | 792 | CYS |
| 1 | I | 828 | ARG |
| 1 | I | 857 | SER |
| 1 | I | 861 | LEU |
| 1 | I | 869 | ASN |
| 1 | I | 872 | LEU |
| 1 | I | 885 | LEU |
| 1 | I | 915 | ASN |
| 1 | I | 924 | ASP |
| 1 | I | 965 | GLU |
| 1 | I | 1061 | LEU |
| 1 | J | 670 | LEU |
| 1 | J | 681 | ILE |
| 1 | J | 692 | SER |
| 1 | J | 719 | GLN |
| 1 | J | 739 | ARG |
| 1 | J | 802 | LEU |
| 1 | J | 828 | ARG |
| 1 | J | 847 | ARG |
| 1 | J | 857 | SER |
| 1 | J | 861 | LEU |
| 1 | J | 872 | LEU |
| 1 | J | 885 | LEU |
| 1 | J | 900 | ASP |
| 1 | J | 910 | ASN |
| 1 | J | 911 | ASP |
| 1 | J | 933 | ILE |
| 1 | J | 935 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | J | 947 | LEU |
| 1 | J | 1015 | GLU |
| 1 | J | 1018 | GLU |
| 1 | J | 1057 | ILE |
| 1 | K | 670 | LEU |
| 1 | K | 686 | GLU |
| 1 | K | 694 | ARG |
| 1 | K | 706 | ASP |
| 1 | K | 719 | GLN |
| 1 | K | 755 | ARG |
| 1 | K | 762 | GLN |
| 1 | K | 792 | CYS |
| 1 | K | 828 | ARG |
| 1 | K | 857 | SER |
| 1 | K | 861 | LEU |
| 1 | K | 869 | ASN |
| 1 | K | 872 | LEU |
| 1 | K | 885 | LEU |
| 1 | K | 915 | ASN |
| 1 | K | 924 | ASP |
| 1 | K | 965 | GLU |
| 1 | K | 1061 | LEU |
| 1 | L | 670 | LEU |
| 1 | L | 681 | ILE |
| 1 | L | 692 | SER |
| 1 | L | 719 | GLN |
| 1 | L | 739 | ARG |
| 1 | L | 802 | LEU |
| 1 | L | 828 | ARG |
| 1 | L | 847 | ARG |
| 1 | L | 857 | SER |
| 1 | L | 861 | LEU |
| 1 | L | 872 | LEU |
| 1 | L | 885 | LEU |
| 1 | L | 900 | ASP |
| 1 | L | 910 | ASN |
| 1 | L | 911 | ASP |
| 1 | L | 933 | ILE |
| 1 | L | 935 | LEU |
| 1 | L | 947 | LEU |
| 1 | L | 1015 | GLU |
| 1 | L | 1021 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L | 1057 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 705 | GLN |
| 1 | A | 719 | GLN |
| 1 | A | 722 | ASN |
| 1 | A | 737 | HIS |
| 1 | A | 762 | GLN |
| 1 | A | 805 | ASN |
| 1 | A | 825 | HIS |
| 1 | A | 869 | ASN |
| 1 | A | 915 | ASN |
| 1 | A | 923 | ASN |
| 1 | A | 939 | ASN |
| 1 | A | 957 | ASN |
| 1 | A | 988 | GLN |
| 1 | A | 994 | HIS |
| 1 | B | 719 | GLN |
| 1 | B | 737 | HIS |
| 1 | B | 805 | ASN |
| 1 | B | 825 | HIS |
| 1 | B | 869 | ASN |
| 1 | B | 915 | ASN |
| 1 | B | 923 | ASN |
| 1 | B | 939 | ASN |
| 1 | C | 718 | GLN |
| 1 | C | 719 | GLN |
| 1 | C | 722 | ASN |
| 1 | C | 737 | HIS |
| 1 | C | 762 | GLN |
| 1 | C | 805 | ASN |
| 1 | C | 825 | HIS |
| 1 | C | 869 | ASN |
| 1 | C | 915 | ASN |
| 1 | C | 923 | ASN |
| 1 | C | 939 | ASN |
| 1 | C | 957 | ASN |
| 1 | C | 988 | GLN |
| 1 | C | 994 | HIS |
| 1 | D | 719 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 737 | HIS |
| 1 | D | 805 | ASN |
| 1 | D | 825 | HIS |
| 1 | D | 869 | ASN |
| 1 | D | 915 | ASN |
| 1 | D | 923 | ASN |
| 1 | D | 939 | ASN |
| 1 | D | 1020 | ASN |
| 1 | E | 718 | GLN |
| 1 | E | 719 | GLN |
| 1 | E | 722 | ASN |
| 1 | E | 737 | HIS |
| 1 | E | 762 | GLN |
| 1 | E | 805 | ASN |
| 1 | E | 825 | HIS |
| 1 | E | 869 | ASN |
| 1 | E | 915 | ASN |
| 1 | E | 923 | ASN |
| 1 | E | 939 | ASN |
| 1 | E | 957 | ASN |
| 1 | E | 988 | GLN |
| 1 | F | 719 | GLN |
| 1 | F | 737 | HIS |
| 1 | F | 805 | ASN |
| 1 | F | 825 | HIS |
| 1 | F | 869 | ASN |
| 1 | F | 923 | ASN |
| 1 | F | 939 | ASN |
| 1 | G | 718 | GLN |
| 1 | G | 719 | GLN |
| 1 | G | 722 | ASN |
| 1 | G | 737 | HIS |
| 1 | G | 762 | GLN |
| 1 | G | 805 | ASN |
| 1 | G | 825 | HIS |
| 1 | G | 869 | ASN |
| 1 | G | 913 | ASN |
| 1 | G | 915 | ASN |
| 1 | G | 923 | ASN |
| 1 | G | 939 | ASN |
| 1 | G | 957 | ASN |
| 1 | G | 988 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | H | 719 | GLN |
| 1 | H | 737 | HIS |
| 1 | H | 794 | ASN |
| 1 | H | 805 | ASN |
| 1 | H | 825 | HIS |
| 1 | H | 869 | ASN |
| 1 | H | 923 | ASN |
| 1 | H | 939 | ASN |
| 1 | I | 718 | GLN |
| 1 | I | 719 | GLN |
| 1 | I | 722 | ASN |
| 1 | I | 737 | HIS |
| 1 | I | 762 | GLN |
| 1 | I | 805 | ASN |
| 1 | I | 825 | HIS |
| 1 | I | 869 | ASN |
| 1 | I | 915 | ASN |
| 1 | I | 923 | ASN |
| 1 | I | 939 | ASN |
| 1 | I | 957 | ASN |
| 1 | I | 988 | GLN |
| 1 | J | 719 | GLN |
| 1 | J | 737 | HIS |
| 1 | J | 805 | ASN |
| 1 | J | 825 | HIS |
| 1 | J | 869 | ASN |
| 1 | J | 923 | ASN |
| 1 | J | 939 | ASN |
| 1 | J | 1063 | HIS |
| 1 | K | 718 | GLN |
| 1 | K | 719 | GLN |
| 1 | K | 722 | ASN |
| 1 | K | 737 | HIS |
| 1 | K | 762 | GLN |
| 1 | K | 794 | ASN |
| 1 | K | 805 | ASN |
| 1 | K | 825 | HIS |
| 1 | K | 869 | ASN |
| 1 | K | 913 | ASN |
| 1 | K | 915 | ASN |
| 1 | K | 923 | ASN |
| 1 | K | 939 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 957 | ASN |
| 1 | K | 988 | GLN |
| 1 | L | 719 | GLN |
| 1 | L | 737 | HIS |
| 1 | L | 805 | ASN |
| 1 | L | 825 | HIS |
| 1 | L | 869 | ASN |
| 1 | L | 915 | ASN |
| 1 | L | 923 | ASN |
| 1 | L | 939 | ASN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|-------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 3 | IBM | A | 2111 | - | 17,17,17 | 2.18 | 5 (29%) | 20,25,25 | 13.27 | 5 (25%) |
| 3 | IBM | B | 2112 | - | 17,17,17 | 2.12 | 5 (29%) | 20,25,25 | 15.12 | 5 (25%) |
| 3 | IBM | C | 2113 | - | 17,17,17 | 2.21 | 5 (29%) | 20,25,25 | 11.21 | 5 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|-------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | IBM | D | 2114 | - | 17,17,17 | 2.37 | 7 (41%) | 20,25,25 | 12.36 | 6 (30%) |
| 3 | IBM | E | 2115 | - | 17,17,17 | 2.10 | 6 (35%) | 20,25,25 | 14.16 | 5 (25%) |
| 3 | IBM | F | 2116 | - | 17,17,17 | 2.00 | 4 (23%) | 20,25,25 | 13.59 | 5 (25%) |
| 3 | IBM | G | 2117 | - | 17,17,17 | 2.16 | 5 (29%) | 20,25,25 | 11.95 | 5 (25%) |
| 3 | IBM | H | 2118 | - | 17,17,17 | 2.24 | 6 (35%) | 20,25,25 | 12.79 | 5 (25%) |
| 3 | IBM | I | 2119 | - | 17,17,17 | 2.19 | 5 (29%) | 20,25,25 | 11.59 | 4 (20%) |
| 3 | IBM | J | 2120 | - | 17,17,17 | 2.19 | 6 (35%) | 20,25,25 | 13.10 | 5 (25%) |
| 3 | IBM | K | 2121 | - | 17,17,17 | 2.22 | 6 (35%) | 20,25,25 | 14.60 | 5 (25%) |
| 3 | IBM | L | 2122 | - | 17,17,17 | 2.28 | 6 (35%) | 20,25,25 | 14.20 | 6 (30%) |

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 |
|-----|------|-------|------|------|---------|----------|---------|
| 3 | IBM | A | 2111 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | B | 2112 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | C | 2113 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | D | 2114 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | E | 2115 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | F | 2116 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | G | 2117 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | H | 2118 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | I | 2119 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | J | 2120 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | K | 2121 | - | - | 0/4/4/4 | 0/0/2/2 |
| 3 | IBM | L | 2122 | - | - | 0/4/4/4 | 0/0/2/2 |

All (66) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3 | C | 2113 | IBM | C6-C5 | 5.51 | 1.50 | 1.41 |
| 3 | D | 2114 | IBM | C6-C5 | 5.49 | 1.50 | 1.41 |
| 3 | J | 2120 | IBM | C6-C5 | 5.48 | 1.50 | 1.41 |
| 3 | G | 2117 | IBM | C6-C5 | 5.37 | 1.50 | 1.41 |
| 3 | I | 2119 | IBM | C6-C5 | 5.33 | 1.49 | 1.41 |
| 3 | H | 2118 | IBM | C6-C5 | 5.25 | 1.49 | 1.41 |
| 3 | A | 2111 | IBM | C4-N3 | 5.06 | 1.49 | 1.38 |
| 3 | L | 2122 | IBM | C6-C5 | 5.00 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3 | E | 2115 | IBM | C6-C5 | 4.86 | 1.49 | 1.41 |
| 3 | K | 2121 | IBM | C6-C5 | 4.82 | 1.49 | 1.41 |
| 3 | K | 2121 | IBM | C4-N3 | 4.74 | 1.49 | 1.38 |
| 3 | F | 2116 | IBM | C6-C5 | 4.67 | 1.48 | 1.41 |
| 3 | L | 2122 | IBM | C4-N3 | 4.64 | 1.48 | 1.38 |
| 3 | A | 2111 | IBM | C6-C5 | 4.63 | 1.48 | 1.41 |
| 3 | E | 2115 | IBM | C4-N3 | 4.62 | 1.48 | 1.38 |
| 3 | C | 2113 | IBM | C4-N3 | 4.51 | 1.48 | 1.38 |
| 3 | D | 2114 | IBM | C4-N3 | 4.44 | 1.48 | 1.38 |
| 3 | G | 2117 | IBM | C4-N3 | 4.40 | 1.48 | 1.38 |
| 3 | B | 2112 | IBM | C6-C5 | 4.31 | 1.48 | 1.41 |
| 3 | B | 2112 | IBM | C4-N3 | 4.30 | 1.48 | 1.38 |
| 3 | I | 2119 | IBM | C4-N3 | 4.26 | 1.48 | 1.38 |
| 3 | H | 2118 | IBM | C4-N3 | 4.23 | 1.47 | 1.38 |
| 3 | J | 2120 | IBM | C4-N3 | 4.22 | 1.47 | 1.38 |
| 3 | F | 2116 | IBM | C4-N3 | 4.05 | 1.47 | 1.38 |
| 3 | L | 2122 | IBM | C2-N1 | 3.62 | 1.42 | 1.38 |
| 3 | D | 2114 | IBM | C2-N1 | 3.43 | 1.42 | 1.38 |
| 3 | C | 2113 | IBM | C5-C4 | -3.18 | 1.33 | 1.40 |
| 3 | A | 2111 | IBM | C5-C4 | -3.18 | 1.33 | 1.40 |
| 3 | H | 2118 | IBM | C2-N1 | 3.11 | 1.41 | 1.38 |
| 3 | J | 2120 | IBM | C5-C4 | -3.07 | 1.33 | 1.40 |
| 3 | I | 2119 | IBM | C11-C12 | 3.06 | 1.56 | 1.52 |
| 3 | B | 2112 | IBM | C5-C4 | -3.04 | 1.33 | 1.40 |
| 3 | I | 2119 | IBM | C5-C4 | -3.02 | 1.33 | 1.40 |
| 3 | K | 2121 | IBM | C11-C12 | 2.99 | 1.56 | 1.52 |
| 3 | D | 2114 | IBM | C2-N3 | 2.92 | 1.41 | 1.38 |
| 3 | K | 2121 | IBM | C5-C4 | -2.89 | 1.34 | 1.40 |
| 3 | F | 2116 | IBM | C5-C4 | -2.89 | 1.34 | 1.40 |
| 3 | H | 2118 | IBM | C5-C4 | -2.86 | 1.34 | 1.40 |
| 3 | D | 2114 | IBM | C5-C4 | -2.83 | 1.34 | 1.40 |
| 3 | B | 2112 | IBM | C2-N3 | 2.82 | 1.41 | 1.38 |
| 3 | B | 2112 | IBM | C2-N1 | 2.81 | 1.41 | 1.38 |
| 3 | L | 2122 | IBM | C5-C4 | -2.67 | 1.34 | 1.40 |
| 3 | A | 2111 | IBM | C11-C12 | 2.65 | 1.56 | 1.52 |
| 3 | G | 2117 | IBM | C5-C4 | -2.62 | 1.34 | 1.40 |
| 3 | F | 2116 | IBM | C2-N3 | 2.57 | 1.41 | 1.38 |
| 3 | E | 2115 | IBM | C2-N1 | 2.53 | 1.41 | 1.38 |
| 3 | H | 2118 | IBM | C11-C12 | 2.53 | 1.56 | 1.52 |
| 3 | K | 2121 | IBM | C2-N3 | 2.53 | 1.41 | 1.38 |
| 3 | E | 2115 | IBM | C5-C4 | -2.46 | 1.34 | 1.40 |
| 3 | E | 2115 | IBM | C11-C12 | 2.44 | 1.56 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3 | D | 2114 | IBM | C11-C12 | 2.42 | 1.56 | 1.52 |
| 3 | J | 2120 | IBM | C2-N1 | 2.41 | 1.41 | 1.38 |
| 3 | G | 2117 | IBM | C2-N1 | 2.41 | 1.41 | 1.38 |
| 3 | L | 2122 | IBM | C2-N3 | 2.40 | 1.41 | 1.38 |
| 3 | I | 2119 | IBM | C2-N1 | 2.35 | 1.41 | 1.38 |
| 3 | C | 2113 | IBM | C2-N3 | 2.30 | 1.40 | 1.38 |
| 3 | J | 2120 | IBM | C2-N3 | 2.29 | 1.40 | 1.38 |
| 3 | J | 2120 | IBM | C11-C12 | 2.27 | 1.55 | 1.52 |
| 3 | K | 2121 | IBM | C2-N1 | 2.26 | 1.40 | 1.38 |
| 3 | H | 2118 | IBM | C2-N3 | 2.21 | 1.40 | 1.38 |
| 3 | G | 2117 | IBM | C11-C12 | 2.15 | 1.55 | 1.52 |
| 3 | L | 2122 | IBM | C11-C12 | 2.12 | 1.55 | 1.52 |
| 3 | E | 2115 | IBM | C6-N1 | 2.07 | 1.41 | 1.35 |
| 3 | C | 2113 | IBM | C11-C12 | 2.05 | 1.55 | 1.52 |
| 3 | A | 2111 | IBM | C2-N3 | 2.02 | 1.40 | 1.38 |
| 3 | D | 2114 | IBM | C4-N9 | 2.01 | 1.47 | 1.38 |

All (61) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 3 | B | 2112 | IBM | C6-C5-N7 | -66.31 | 130.71 | 134.24 |
| 3 | K | 2121 | IBM | C6-C5-N7 | -63.55 | 130.86 | 134.24 |
| 3 | L | 2122 | IBM | C6-C5-N7 | -61.99 | 130.94 | 134.24 |
| 3 | E | 2115 | IBM | C6-C5-N7 | -61.50 | 130.97 | 134.24 |
| 3 | F | 2116 | IBM | C6-C5-N7 | -59.17 | 131.09 | 134.24 |
| 3 | A | 2111 | IBM | C6-C5-N7 | -57.63 | 131.17 | 134.24 |
| 3 | J | 2120 | IBM | C6-C5-N7 | -56.99 | 131.21 | 134.24 |
| 3 | H | 2118 | IBM | C6-C5-N7 | -55.66 | 131.28 | 134.24 |
| 3 | D | 2114 | IBM | C6-C5-N7 | -53.55 | 131.39 | 134.24 |
| 3 | G | 2117 | IBM | C6-C5-N7 | -51.69 | 131.49 | 134.24 |
| 3 | I | 2119 | IBM | C6-C5-N7 | -50.02 | 131.58 | 134.24 |
| 3 | C | 2113 | IBM | C6-C5-N7 | -48.27 | 131.67 | 134.24 |
| 3 | E | 2115 | IBM | N9-C4-N3 | 13.03 | 131.75 | 127.55 |
| 3 | K | 2121 | IBM | N9-C4-N3 | 12.95 | 131.73 | 127.55 |
| 3 | A | 2111 | IBM | N9-C4-N3 | 11.91 | 131.39 | 127.55 |
| 3 | L | 2122 | IBM | N9-C4-N3 | 11.50 | 131.26 | 127.55 |
| 3 | F | 2116 | IBM | N9-C4-N3 | 11.08 | 131.12 | 127.55 |
| 3 | H | 2118 | IBM | N9-C4-N3 | 11.04 | 131.11 | 127.55 |
| 3 | I | 2119 | IBM | N9-C4-N3 | 11.04 | 131.11 | 127.55 |
| 3 | C | 2113 | IBM | N9-C4-N3 | 10.87 | 131.06 | 127.55 |
| 3 | G | 2117 | IBM | N9-C4-N3 | 10.87 | 131.06 | 127.55 |
| 3 | J | 2120 | IBM | N9-C4-N3 | 10.84 | 131.05 | 127.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3 | D | 2114 | IBM | N9-C4-N3 | 10.82 | 131.04 | 127.55 |
| 3 | B | 2112 | IBM | N9-C4-N3 | 10.76 | 131.02 | 127.55 |
| 3 | J | 2120 | IBM | C6-N1-C2 | 6.96 | 124.13 | 121.69 |
| 3 | F | 2116 | IBM | C6-N1-C2 | 6.66 | 124.02 | 121.69 |
| 3 | G | 2117 | IBM | C6-N1-C2 | 6.60 | 124.00 | 121.69 |
| 3 | I | 2119 | IBM | C6-N1-C2 | 6.59 | 124.00 | 121.69 |
| 3 | D | 2114 | IBM | C6-N1-C2 | 6.29 | 123.89 | 121.69 |
| 3 | K | 2121 | IBM | C6-N1-C2 | 6.27 | 123.89 | 121.69 |
| 3 | A | 2111 | IBM | C6-N1-C2 | 6.24 | 123.88 | 121.69 |
| 3 | C | 2113 | IBM | C6-N1-C2 | 6.19 | 123.86 | 121.69 |
| 3 | L | 2122 | IBM | C6-N1-C2 | 5.98 | 123.78 | 121.69 |
| 3 | B | 2112 | IBM | C6-N1-C2 | 5.96 | 123.78 | 121.69 |
| 3 | H | 2118 | IBM | C6-N1-C2 | 5.87 | 123.75 | 121.69 |
| 3 | E | 2115 | IBM | C6-N1-C2 | 5.76 | 123.70 | 121.69 |
| 3 | C | 2113 | IBM | C5-C4-N9 | 3.40 | 109.40 | 106.07 |
| 3 | B | 2112 | IBM | C5-C4-N9 | 3.26 | 109.26 | 106.07 |
| 3 | G | 2117 | IBM | C5-C4-N9 | 3.21 | 109.21 | 106.07 |
| 3 | H | 2118 | IBM | C5-C4-N9 | 3.20 | 109.20 | 106.07 |
| 3 | F | 2116 | IBM | C5-C4-N9 | 3.20 | 109.20 | 106.07 |
| 3 | J | 2120 | IBM | C5-C4-N9 | 3.10 | 109.10 | 106.07 |
| 3 | I | 2119 | IBM | C5-C4-N9 | 3.06 | 109.06 | 106.07 |
| 3 | E | 2115 | IBM | C5-C4-N9 | 2.99 | 108.99 | 106.07 |
| 3 | L | 2122 | IBM | C5-C4-N9 | 2.95 | 108.95 | 106.07 |
| 3 | A | 2111 | IBM | C5-C4-N9 | 2.95 | 108.95 | 106.07 |
| 3 | D | 2114 | IBM | C11-N3-C4 | -2.94 | 115.99 | 118.93 |
| 3 | D | 2114 | IBM | C5-C4-N9 | 2.93 | 108.93 | 106.07 |
| 3 | K | 2121 | IBM | C5-C4-N9 | 2.71 | 108.72 | 106.07 |
| 3 | L | 2122 | IBM | C12-C11-N3 | 2.33 | 115.75 | 112.38 |
| 3 | F | 2116 | IBM | C8-N9-C4 | -2.33 | 102.82 | 107.10 |
| 3 | E | 2115 | IBM | C8-N9-C4 | -2.27 | 102.92 | 107.10 |
| 3 | B | 2112 | IBM | C8-N9-C4 | -2.27 | 102.93 | 107.10 |
| 3 | G | 2117 | IBM | C8-N9-C4 | -2.22 | 103.02 | 107.10 |
| 3 | C | 2113 | IBM | C8-N9-C4 | -2.17 | 103.10 | 107.10 |
| 3 | A | 2111 | IBM | C8-N9-C4 | -2.16 | 103.14 | 107.10 |
| 3 | H | 2118 | IBM | C8-N9-C4 | -2.08 | 103.28 | 107.10 |
| 3 | J | 2120 | IBM | C8-N9-C4 | -2.06 | 103.31 | 107.10 |
| 3 | K | 2121 | IBM | C8-N9-C4 | -2.06 | 103.32 | 107.10 |
| 3 | L | 2122 | IBM | C8-N9-C4 | -2.05 | 103.32 | 107.10 |
| 3 | D | 2114 | IBM | C8-N9-C4 | -2.02 | 103.39 | 107.10 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 | 364/420 (86%) | 0.04 | 11 (3%) | 48 | 57 | 24, 42, 80, 100 | 0 |
| 1 | B | 381/420 (90%) | 0.37 | 30 (7%) | 13 | 15 | 25, 50, 92, 100 | 0 |
| 1 | C | 364/420 (86%) | 0.16 | 18 (4%) | 28 | 34 | 26, 43, 81, 100 | 0 |
| 1 | D | 381/420 (90%) | 0.40 | 29 (7%) | 14 | 17 | 22, 47, 89, 100 | 0 |
| 1 | E | 364/420 (86%) | 0.12 | 15 (4%) | 35 | 43 | 23, 42, 81, 100 | 0 |
| 1 | F | 381/420 (90%) | 0.19 | 16 (4%) | 35 | 41 | 21, 45, 79, 100 | 0 |
| 1 | G | 364/420 (86%) | 0.05 | 19 (5%) | 26 | 32 | 24, 44, 83, 100 | 0 |
| 1 | H | 381/420 (90%) | 0.30 | 24 (6%) | 19 | 23 | 29, 52, 92, 100 | 0 |
| 1 | I | 364/420 (86%) | 0.12 | 16 (4%) | 33 | 40 | 23, 42, 81, 100 | 0 |
| 1 | J | 381/420 (90%) | 0.14 | 10 (2%) | 53 | 63 | 22, 46, 77, 100 | 0 |
| 1 | K | 364/420 (86%) | 0.68 | 65 (17%) | 2 | 3 | 28, 51, 87, 100 | 0 |
| 1 | L | 381/420 (90%) | 0.57 | 37 (9%) | 8 | 10 | 29, 54, 91, 100 | 0 |
| All | All | 4470/5040 (88%) | 0.26 | 290 (6%) | 18 | 22 | 21, 46, 85, 100 | 0 |

All (290) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 659 | LEU | 13.0 |
| 1 | B | 1053 | SER | 11.7 |
| 1 | H | 1022 | THR | 11.4 |
| 1 | C | 1016 | ALA | 11.3 |
| 1 | B | 1024 | SER | 11.2 |
| 1 | H | 1016 | ALA | 11.0 |
| 1 | E | 1016 | ALA | 10.9 |
| 1 | K | 1053 | SER | 10.8 |
| 1 | L | 1016 | ALA | 10.7 |
| 1 | L | 1053 | SER | 10.5 |
| 1 | D | 657 | VAL | 10.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | H | 1018 | GLU | 10.4 |
| 1 | H | 1020 | ASN | 10.3 |
| 1 | D | 1021 | ASP | 10.3 |
| 1 | L | 1021 | ASP | 10.2 |
| 1 | D | 1053 | SER | 10.2 |
| 1 | B | 1022 | THR | 10.0 |
| 1 | B | 1021 | ASP | 9.7 |
| 1 | I | 1016 | ALA | 9.4 |
| 1 | H | 1021 | ASP | 9.1 |
| 1 | B | 1018 | GLU | 8.9 |
| 1 | L | 1020 | ASN | 8.8 |
| 1 | B | 1019 | ASP | 8.8 |
| 1 | D | 1024 | SER | 8.8 |
| 1 | H | 1024 | SER | 8.7 |
| 1 | L | 1022 | THR | 8.7 |
| 1 | A | 1016 | ALA | 8.7 |
| 1 | I | 1053 | SER | 8.6 |
| 1 | B | 1016 | ALA | 8.5 |
| 1 | D | 1019 | ASP | 8.5 |
| 1 | D | 658 | SER | 8.5 |
| 1 | A | 1053 | SER | 8.3 |
| 1 | D | 1016 | ALA | 8.2 |
| 1 | H | 1019 | ASP | 8.2 |
| 1 | B | 1023 | GLU | 8.1 |
| 1 | B | 1020 | ASN | 8.1 |
| 1 | D | 1022 | THR | 8.0 |
| 1 | L | 1017 | GLU | 8.0 |
| 1 | C | 1017 | GLU | 7.9 |
| 1 | B | 1054 | ARG | 7.9 |
| 1 | D | 1018 | GLU | 7.8 |
| 1 | A | 1017 | GLU | 7.8 |
| 1 | L | 1018 | GLU | 7.8 |
| 1 | D | 1020 | ASN | 7.7 |
| 1 | L | 1023 | GLU | 7.6 |
| 1 | K | 1017 | GLU | 7.5 |
| 1 | B | 657 | VAL | 7.5 |
| 1 | L | 1054 | ARG | 7.5 |
| 1 | G | 1053 | SER | 7.5 |
| 1 | D | 1017 | GLU | 7.5 |
| 1 | G | 1016 | ALA | 7.5 |
| 1 | D | 1023 | GLU | 7.5 |
| 1 | F | 658 | SER | 7.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | L | 1019 | ASP | 7.4 |
| 1 | F | 656 | GLU | 7.4 |
| 1 | L | 1024 | SER | 7.2 |
| 1 | H | 658 | SER | 7.1 |
| 1 | C | 1053 | SER | 6.9 |
| 1 | H | 1053 | SER | 6.9 |
| 1 | L | 657 | VAL | 6.8 |
| 1 | J | 657 | VAL | 6.8 |
| 1 | D | 660 | ASP | 6.7 |
| 1 | H | 1017 | GLU | 6.7 |
| 1 | I | 1054 | ARG | 6.6 |
| 1 | L | 656 | GLU | 6.5 |
| 1 | H | 656 | GLU | 6.4 |
| 1 | E | 1017 | GLU | 6.4 |
| 1 | I | 1017 | GLU | 6.2 |
| 1 | A | 766 | GLY | 6.2 |
| 1 | K | 1016 | ALA | 6.2 |
| 1 | B | 658 | SER | 6.1 |
| 1 | E | 659 | LEU | 6.1 |
| 1 | B | 1017 | GLU | 6.1 |
| 1 | L | 658 | SER | 6.0 |
| 1 | D | 1054 | ARG | 6.0 |
| 1 | G | 1017 | GLU | 6.0 |
| 1 | B | 656 | GLU | 5.9 |
| 1 | F | 657 | VAL | 5.9 |
| 1 | L | 659 | LEU | 5.8 |
| 1 | D | 659 | LEU | 5.8 |
| 1 | H | 1054 | ARG | 5.7 |
| 1 | H | 659 | LEU | 5.6 |
| 1 | I | 764 | HIS | 5.6 |
| 1 | H | 1023 | GLU | 5.5 |
| 1 | J | 658 | SER | 5.5 |
| 1 | F | 659 | LEU | 5.5 |
| 1 | H | 657 | VAL | 5.4 |
| 1 | J | 660 | ASP | 5.4 |
| 1 | C | 765 | ASN | 5.3 |
| 1 | E | 1053 | SER | 5.3 |
| 1 | C | 660 | ASP | 5.3 |
| 1 | J | 656 | GLU | 5.2 |
| 1 | H | 1015 | GLU | 5.1 |
| 1 | L | 1015 | GLU | 5.1 |
| 1 | E | 765 | ASN | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | K | 1014 | LEU | 5.1 |
| 1 | K | 1056 | ARG | 5.1 |
| 1 | E | 766 | GLY | 5.0 |
| 1 | C | 766 | GLY | 5.0 |
| 1 | L | 765 | ASN | 4.9 |
| 1 | G | 913 | ASN | 4.9 |
| 1 | D | 662 | ILE | 4.9 |
| 1 | I | 659 | LEU | 4.8 |
| 1 | F | 1019 | ASP | 4.8 |
| 1 | G | 764 | HIS | 4.8 |
| 1 | D | 661 | LEU | 4.8 |
| 1 | G | 765 | ASN | 4.7 |
| 1 | C | 764 | HIS | 4.7 |
| 1 | E | 660 | ASP | 4.6 |
| 1 | K | 701 | TYR | 4.6 |
| 1 | D | 656 | GLU | 4.6 |
| 1 | K | 761 | GLN | 4.6 |
| 1 | A | 1054 | ARG | 4.5 |
| 1 | F | 1053 | SER | 4.5 |
| 1 | K | 659 | LEU | 4.4 |
| 1 | B | 660 | ASP | 4.4 |
| 1 | I | 766 | GLY | 4.3 |
| 1 | E | 764 | HIS | 4.3 |
| 1 | L | 1055 | ARG | 4.3 |
| 1 | D | 1015 | GLU | 4.2 |
| 1 | L | 660 | ASP | 4.2 |
| 1 | G | 1054 | ARG | 4.2 |
| 1 | K | 1054 | ARG | 4.2 |
| 1 | K | 802 | LEU | 4.1 |
| 1 | K | 764 | HIS | 4.1 |
| 1 | B | 1015 | GLU | 4.0 |
| 1 | K | 660 | ASP | 4.0 |
| 1 | H | 766 | GLY | 4.0 |
| 1 | L | 763 | ILE | 4.0 |
| 1 | J | 765 | ASN | 4.0 |
| 1 | B | 659 | LEU | 4.0 |
| 1 | K | 1055 | ARG | 3.9 |
| 1 | K | 1057 | ILE | 3.9 |
| 1 | I | 660 | ASP | 3.9 |
| 1 | L | 912 | VAL | 3.9 |
| 1 | J | 659 | LEU | 3.9 |
| 1 | J | 1053 | SER | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | L | 764 | HIS | 3.8 |
| 1 | C | 661 | LEU | 3.8 |
| 1 | B | 766 | GLY | 3.7 |
| 1 | K | 1012 | GLN | 3.7 |
| 1 | B | 1055 | ARG | 3.6 |
| 1 | K | 795 | PRO | 3.6 |
| 1 | L | 1014 | LEU | 3.6 |
| 1 | F | 660 | ASP | 3.5 |
| 1 | K | 787 | ILE | 3.5 |
| 1 | F | 912 | VAL | 3.5 |
| 1 | K | 763 | ILE | 3.5 |
| 1 | L | 1013 | TRP | 3.5 |
| 1 | K | 815 | TYR | 3.5 |
| 1 | H | 660 | ASP | 3.5 |
| 1 | F | 1020 | ASN | 3.4 |
| 1 | E | 661 | LEU | 3.4 |
| 1 | F | 1018 | GLU | 3.4 |
| 1 | L | 766 | GLY | 3.4 |
| 1 | D | 765 | ASN | 3.3 |
| 1 | G | 784 | ILE | 3.3 |
| 1 | E | 1054 | ARG | 3.2 |
| 1 | G | 663 | LEU | 3.2 |
| 1 | C | 1015 | GLU | 3.2 |
| 1 | I | 765 | ASN | 3.2 |
| 1 | K | 1015 | GLU | 3.2 |
| 1 | G | 912 | VAL | 3.1 |
| 1 | B | 765 | ASN | 3.1 |
| 1 | H | 1055 | ARG | 3.1 |
| 1 | C | 662 | ILE | 3.1 |
| 1 | K | 704 | PHE | 3.0 |
| 1 | K | 916 | GLY | 3.0 |
| 1 | D | 763 | ILE | 3.0 |
| 1 | K | 699 | VAL | 2.9 |
| 1 | K | 717 | THR | 2.9 |
| 1 | K | 800 | GLY | 2.9 |
| 1 | K | 720 | PHE | 2.9 |
| 1 | G | 766 | GLY | 2.9 |
| 1 | H | 913 | ASN | 2.9 |
| 1 | K | 806 | ILE | 2.9 |
| 1 | A | 659 | LEU | 2.9 |
| 1 | J | 1020 | ASN | 2.8 |
| 1 | C | 663 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | G | 660 | ASP | 2.8 |
| 1 | K | 757 | VAL | 2.8 |
| 1 | A | 765 | ASN | 2.8 |
| 1 | I | 1056 | ARG | 2.8 |
| 1 | G | 664 | VAL | 2.8 |
| 1 | K | 919 | TRP | 2.8 |
| 1 | F | 662 | ILE | 2.8 |
| 1 | B | 1014 | LEU | 2.8 |
| 1 | B | 661 | LEU | 2.8 |
| 1 | L | 661 | LEU | 2.8 |
| 1 | E | 912 | VAL | 2.7 |
| 1 | B | 1056 | ARG | 2.7 |
| 1 | C | 1054 | ARG | 2.7 |
| 1 | K | 765 | ASN | 2.7 |
| 1 | G | 1056 | ARG | 2.7 |
| 1 | D | 663 | LEU | 2.7 |
| 1 | H | 764 | HIS | 2.7 |
| 1 | C | 761 | GLN | 2.7 |
| 1 | K | 705 | GLN | 2.6 |
| 1 | D | 1014 | LEU | 2.6 |
| 1 | K | 762 | GLN | 2.6 |
| 1 | H | 912 | VAL | 2.6 |
| 1 | K | 1013 | TRP | 2.6 |
| 1 | I | 761 | GLN | 2.6 |
| 1 | E | 913 | ASN | 2.6 |
| 1 | K | 913 | ASN | 2.6 |
| 1 | I | 912 | VAL | 2.6 |
| 1 | B | 912 | VAL | 2.6 |
| 1 | F | 661 | LEU | 2.5 |
| 1 | K | 1058 | PHE | 2.5 |
| 1 | I | 662 | ILE | 2.5 |
| 1 | D | 766 | GLY | 2.5 |
| 1 | E | 662 | ILE | 2.5 |
| 1 | K | 662 | ILE | 2.5 |
| 1 | K | 1009 | LEU | 2.4 |
| 1 | L | 994 | HIS | 2.4 |
| 1 | E | 665 | GLU | 2.4 |
| 1 | A | 916 | GLY | 2.4 |
| 1 | K | 1010 | PRO | 2.4 |
| 1 | E | 916 | GLY | 2.4 |
| 1 | K | 663 | LEU | 2.4 |
| 1 | B | 663 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | K | 805 | ASN | 2.4 |
| 1 | F | 1021 | ASP | 2.4 |
| 1 | L | 969 | LEU | 2.4 |
| 1 | K | 1011 | GLY | 2.4 |
| 1 | L | 663 | LEU | 2.4 |
| 1 | F | 765 | ASN | 2.4 |
| 1 | J | 1000 | CYS | 2.4 |
| 1 | K | 766 | GLY | 2.3 |
| 1 | H | 1014 | LEU | 2.3 |
| 1 | K | 1003 | TYR | 2.3 |
| 1 | G | 763 | ILE | 2.3 |
| 1 | G | 661 | LEU | 2.3 |
| 1 | L | 1056 | ARG | 2.3 |
| 1 | K | 667 | TYR | 2.3 |
| 1 | K | 915 | ASN | 2.3 |
| 1 | D | 1056 | ARG | 2.3 |
| 1 | K | 703 | LEU | 2.3 |
| 1 | K | 664 | VAL | 2.3 |
| 1 | C | 1014 | LEU | 2.2 |
| 1 | K | 760 | LEU | 2.2 |
| 1 | D | 764 | HIS | 2.2 |
| 1 | K | 758 | PRO | 2.2 |
| 1 | L | 1059 | CYS | 2.2 |
| 1 | K | 709 | LEU | 2.2 |
| 1 | K | 694 | ARG | 2.2 |
| 1 | L | 913 | ASN | 2.2 |
| 1 | D | 761 | GLN | 2.2 |
| 1 | B | 764 | HIS | 2.2 |
| 1 | L | 971 | LEU | 2.2 |
| 1 | A | 784 | ILE | 2.2 |
| 1 | K | 674 | MET | 2.2 |
| 1 | B | 1013 | TRP | 2.2 |
| 1 | L | 978 | ASP | 2.2 |
| 1 | B | 662 | ILE | 2.2 |
| 1 | C | 665 | GLU | 2.2 |
| 1 | F | 664 | VAL | 2.2 |
| 1 | L | 761 | GLN | 2.2 |
| 1 | K | 793 | SER | 2.2 |
| 1 | G | 659 | LEU | 2.2 |
| 1 | J | 1021 | ASP | 2.2 |
| 1 | K | 665 | GLU | 2.1 |
| 1 | K | 912 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | K | 794 | ASN | 2.1 |
| 1 | K | 691 | LYS | 2.1 |
| 1 | L | 662 | ILE | 2.1 |
| 1 | A | 1056 | ARG | 2.1 |
| 1 | K | 700 | MET | 2.1 |
| 1 | K | 750 | TRP | 2.1 |
| 1 | B | 667 | TYR | 2.1 |
| 1 | K | 715 | ILE | 2.1 |
| 1 | I | 1015 | GLU | 2.1 |
| 1 | I | 661 | LEU | 2.1 |
| 1 | C | 913 | ASN | 2.1 |
| 1 | K | 707 | THR | 2.1 |
| 1 | A | 664 | VAL | 2.0 |
| 1 | G | 1055 | ARG | 2.0 |
| 1 | H | 661 | LEU | 2.0 |
| 1 | C | 664 | VAL | 2.0 |
| 1 | D | 912 | VAL | 2.0 |
| 1 | B | 1057 | ILE | 2.0 |
| 1 | D | 695 | ILE | 2.0 |
| 1 | K | 724 | PHE | 2.0 |
| 1 | I | 1014 | LEU | 2.0 |
| 1 | K | 759 | GLY | 2.0 |
| 1 | G | 665 | GLU | 2.0 |
| 1 | K | 784 | ILE | 2.0 |
| 1 | L | 1058 | PHE | 2.0 |
| 1 | F | 766 | GLY | 2.0 |
| 1 | K | 746 | LEU | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th 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 | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 3 | IBM | G | 2117 | 16/16 | 0.22 | 1.78 | 44,49,50,51 | 0 |
| 3 | IBM | H | 2118 | 16/16 | 0.28 | 1.59 | 72,78,79,80 | 0 |
| 3 | IBM | E | 2115 | 16/16 | 0.19 | 1.32 | 28,32,35,37 | 0 |
| 3 | IBM | B | 2112 | 16/16 | 0.25 | 1.22 | 54,56,59,59 | 0 |
| 3 | IBM | C | 2113 | 16/16 | 0.18 | 0.94 | 36,42,48,48 | 0 |
| 3 | IBM | K | 2121 | 16/16 | 0.18 | 0.68 | 54,59,60,61 | 0 |
| 3 | IBM | J | 2120 | 16/16 | 0.23 | 0.59 | 31,35,40,41 | 0 |
| 3 | IBM | D | 2114 | 16/16 | 0.21 | 0.56 | 35,53,56,57 | 0 |
| 3 | IBM | A | 2111 | 16/16 | 0.19 | 0.52 | 36,38,42,42 | 0 |
| 3 | IBM | I | 2119 | 16/16 | 0.19 | 0.38 | 35,38,39,39 | 0 |
| 3 | IBM | L | 2122 | 16/16 | 0.23 | 0.26 | 68,77,78,79 | 0 |
| 2 | MG | C | 2127 | 1/1 | 0.15 | 0.12 | 5,5,5,5 | 0 |
| 2 | MG | H | 2137 | 1/1 | 0.13 | -0.10 | 12,12,12,12 | 0 |
| 2 | MG | I | 2139 | 1/1 | 0.15 | -0.49 | 5,5,5,5 | 0 |
| 2 | MG | L | 2145 | 1/1 | 0.13 | -0.49 | 23,23,23,23 | 0 |
| 2 | MG | F | 2133 | 1/1 | 0.15 | -0.57 | 1,1,1,1 | 0 |
| 2 | MG | D | 2129 | 1/1 | 0.15 | -0.72 | 9,9,9,9 | 0 |
| 2 | MG | K | 2143 | 1/1 | 0.12 | -0.84 | 20,20,20,20 | 0 |
| 3 | IBM | F | 2116 | 16/16 | 0.17 | -0.99 | 28,37,40,40 | 0 |
| 2 | MG | K | 2144 | 1/1 | 0.13 | -1.00 | 40,40,40,40 | 0 |
| 2 | MG | J | 2141 | 1/1 | 0.14 | -1.24 | 6,6,6,6 | 0 |
| 2 | MG | E | 2131 | 1/1 | 0.15 | -1.31 | 1,1,1,1 | 0 |
| 2 | MG | G | 2135 | 1/1 | 0.12 | -1.68 | 1,1,1,1 | 0 |
| 2 | MG | C | 2128 | 1/1 | 0.11 | -1.88 | 29,29,29,29 | 0 |
| 2 | MG | A | 2123 | 1/1 | 0.12 | -1.89 | 2,2,2,2 | 0 |
| 2 | MG | B | 2126 | 1/1 | 0.11 | -2.11 | 56,56,56,56 | 0 |
| 2 | MG | E | 2132 | 1/1 | 0.14 | -2.15 | 29,29,29,29 | 0 |
| 2 | MG | B | 2125 | 1/1 | 0.09 | -2.26 | 4,4,4,4 | 0 |
| 2 | MG | J | 2142 | 1/1 | 0.13 | -2.39 | 39,39,39,39 | 0 |
| 2 | MG | A | 2124 | 1/1 | 0.11 | -2.47 | 41,41,41,41 | 0 |
| 2 | MG | I | 2140 | 1/1 | 0.13 | -2.51 | 27,27,27,27 | 0 |
| 2 | MG | G | 2136 | 1/1 | 0.11 | -2.65 | 28,28,28,28 | 0 |
| 2 | MG | L | 2146 | 1/1 | 0.07 | -3.03 | 30,30,30,30 | 0 |
| 2 | MG | D | 2130 | 1/1 | 0.11 | -3.07 | 22,22,22,22 | 0 |
| 2 | MG | H | 2138 | 1/1 | 0.06 | -3.29 | 32,32,32,32 | 0 |
| 2 | MG | F | 2134 | 1/1 | 0.06 | -5.05 | 19,19,19,19 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.