



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:33 AM UTC

PDB ID : 4Q5V / pdb\_00004q5v  
Title : Crystal structure of the catalytic core of human DNA polymerase alpha in ternary complex with an RNA-primed DNA template and aphidicolin  
Authors : Baranovskiy, A.G.; Babayeva, N.D.; Suwa, Y.; Gu, J.; Tahirov, T.H.  
Deposited on : 2014-04-17  
Resolution : 2.52 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

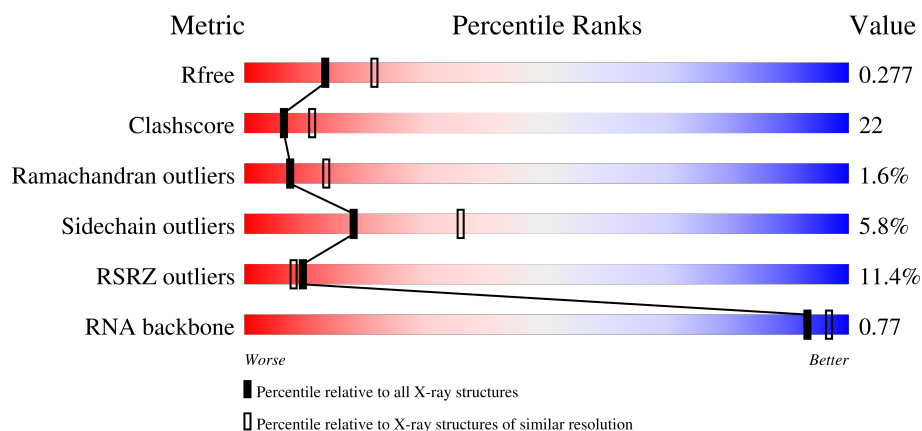
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.52 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 7383 (2.54-2.50)                                      |
| Clashscore            | 190562                      | 8079 (2.54-2.50)                                      |
| Ramachandran outliers | 187476                      | 7944 (2.54-2.50)                                      |
| Sidechain outliers    | 187428                      | 7946 (2.54-2.50)                                      |
| RSRZ outliers         | 180081                      | 7387 (2.54-2.50)                                      |
| RNA backbone          | 3983                        | 1161 (2.80-2.24)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                               |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------|
| 1   | A     | 922    | <div> <div>12%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>5%</div> <div>6%</div> </div> </div> |
| 1   | E     | 922    | <div> <div>10%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>5%</div> <div>6%</div> </div> </div> |
| 2   | B     | 11     | <div> <div>9%</div> <div> <div></div> <div>82%</div> <div>9%</div> </div> </div>                               |
| 2   | F     | 11     | <div> <div>36%</div> <div> <div></div> <div>55%</div> <div>9%</div> </div> </div>                              |

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| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 3   | C     | 21     | <div><div><div>5%</div><div>10%</div><div>48%</div><div>5%</div><div>38%</div></div></div> |
| 3   | G     | 21     | <div><div><div>5%</div><div>10%</div><div>48%</div><div>5%</div><div>38%</div></div></div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA polymerase alpha catalytic subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 865      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6947  | 4470 | 1162 | 1274 | 41 |         |         |       |
| 1   | E     | 865      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6947  | 4470 | 1162 | 1274 | 41 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 516     | ALA      | VAL    | engineered mutation | UNP P09884 |
| E     | 516     | ALA      | VAL    | engineered mutation | UNP P09884 |

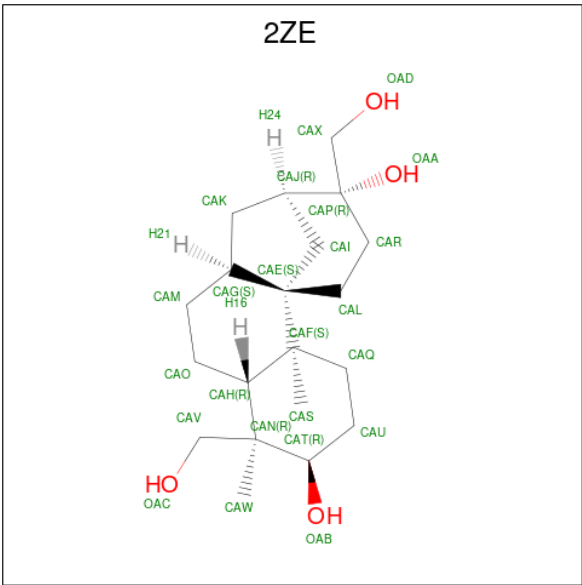
- Molecule 2 is a RNA chain called RNA primer.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 2   | B     | 11       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 232   | 105 | 44 | 73 | 10 |         |         |       |
| 2   | F     | 11       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 232   | 105 | 44 | 73 | 10 |         |         |       |

- Molecule 3 is a DNA chain called DNA template.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 3   | C     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 264   | 125 | 52 | 75 | 12 |         |         |       |
| 3   | G     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 264   | 125 | 52 | 75 | 12 |         |         |       |

- Molecule 4 is (3R,4R,4aR,6aS,8R,9R,11aS,11bS)-4,9-bis(hydroxymethyl)-4,11b-dimethylte tradecahydro-8,11a-methanocyclohepta[a]naphthale ne-3,9-diol (CCD ID: 2ZE) (formula: C<sub>20</sub>H<sub>34</sub>O<sub>4</sub>).

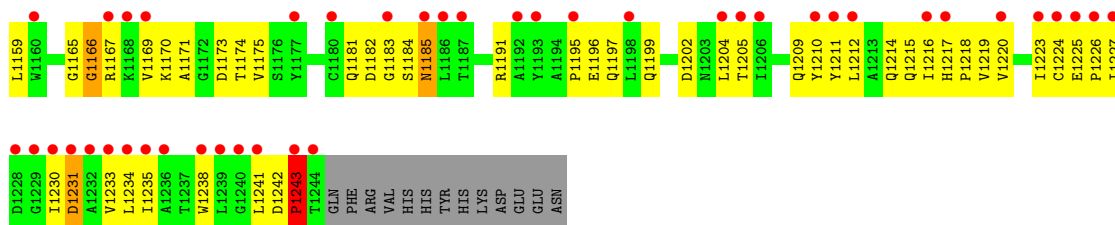


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 24    | 20 | 4 |         |         |
| 4   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 24    | 20 | 4 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 80       | Total | O  | 0       | 0       |
|     |       |          | 80    | 80 |         |         |
| 5   | B     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | C     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 5   | E     | 62       | Total | O  | 0       | 0       |
|     |       |          | 62    | 62 |         |         |
| 5   | F     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 5   | G     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

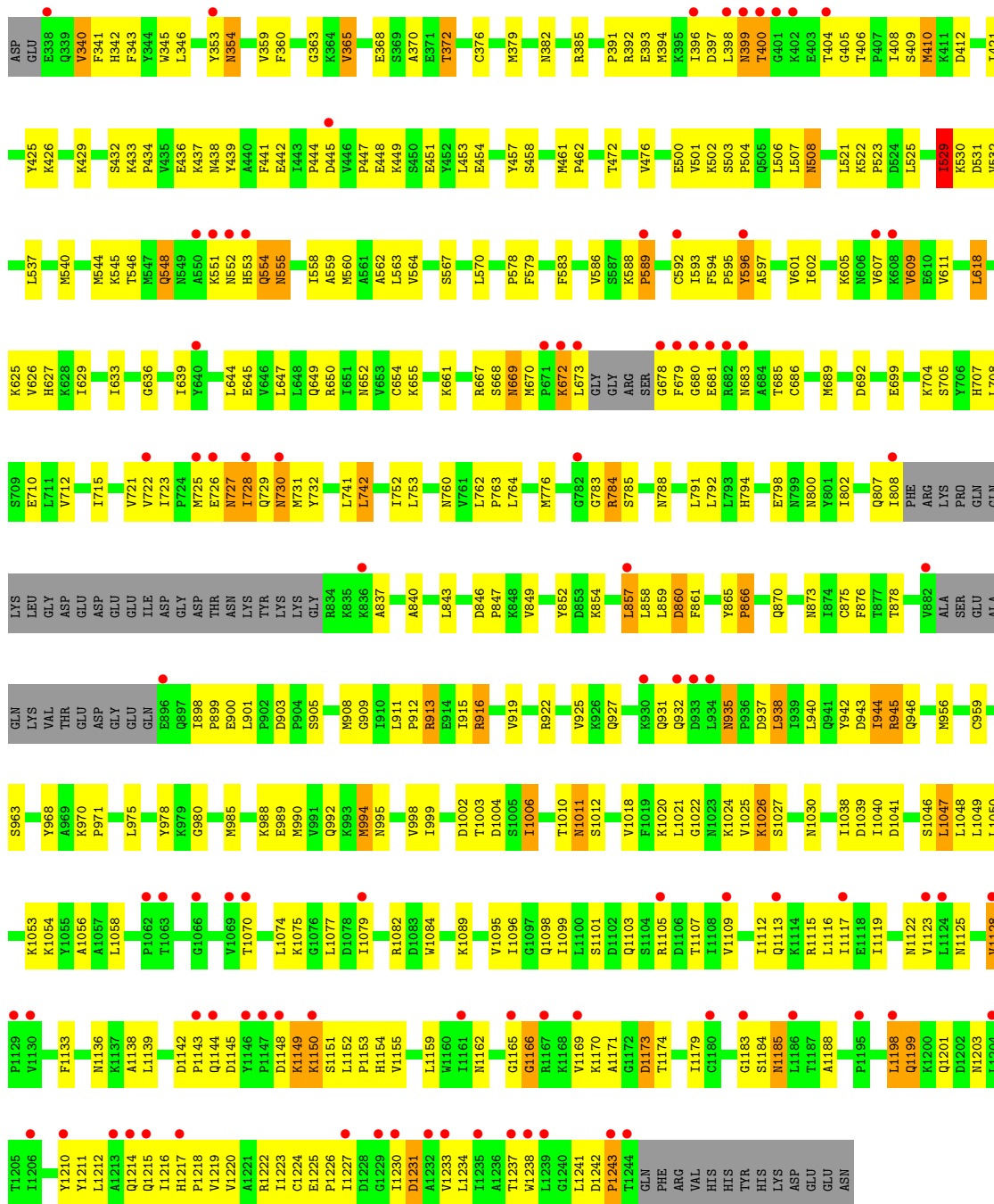




● Molecule 1: DNA polymerase alpha catalytic subunit



Chain E:



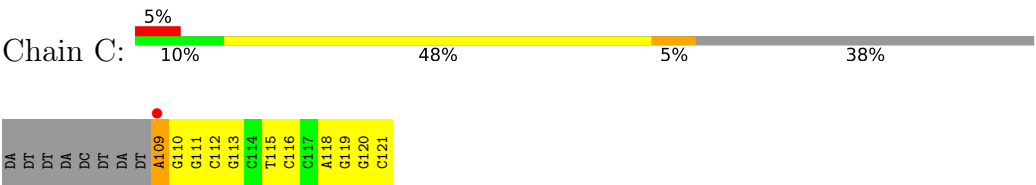
● Molecule 2: RNA primer



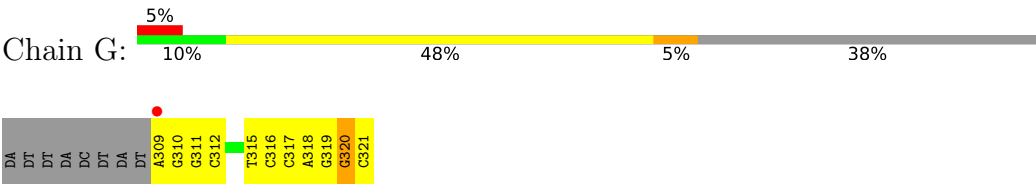
● Molecule 2: RNA primer



● Molecule 3: DNA template



● Molecule 3: DNA template



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 105.05Å 116.43Å 233.03Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 78.02 – 2.52<br>78.02 – 2.52                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.0 (78.02-2.52)<br>96.3 (78.02-2.52)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.04                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 189.48 (at 2.51Å)                                           | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.233 , 0.268<br>0.246 , 0.277                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4714 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 42.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.254                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 45.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 15085                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 59.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2ZE

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     | 0.55         | 2/7089 (0.0%)  | 1.03        | 26/9582 (0.3%)  |
| 1   | E     | 0.56         | 0/7089         | 1.02        | 18/9582 (0.2%)  |
| 2   | B     | 0.35         | 0/259          | 0.91        | 2/402 (0.5%)    |
| 2   | F     | 0.37         | 0/259          | 0.84        | 1/402 (0.2%)    |
| 3   | C     | 0.33         | 0/296          | 0.84        | 1/455 (0.2%)    |
| 3   | G     | 0.33         | 0/296          | 0.82        | 1/455 (0.2%)    |
| All | All   | 0.54         | 2/15288 (0.0%) | 1.01        | 49/20878 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | G     | 0                   | 1                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 689 | MET  | SD-CE | -7.21 | 1.61        | 1.79     |
| 1   | A     | 985 | MET  | SD-CE | 5.08  | 1.92        | 1.79     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 552 | ASN  | N-CA-C | 10.23 | 127.15      | 109.96   |
| 1   | E     | 442 | GLU  | N-CA-C | 10.13 | 125.16      | 113.01   |
| 1   | A     | 553 | HIS  | N-CA-C | 9.80  | 131.67      | 110.80   |
| 1   | A     | 802 | ILE  | N-CA-C | -9.55 | 96.22       | 109.21   |
| 1   | E     | 400 | THR  | N-CA-C | -7.89 | 101.64      | 111.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | C     | 109  | DA   | C2'-C3'-O3' | -7.82 | 99.77       | 111.50   |
| 1   | E     | 802  | ILE  | N-CA-C      | -7.82 | 97.33       | 108.58   |
| 1   | E     | 1183 | GLY  | N-CA-C      | -7.75 | 102.37      | 115.08   |
| 1   | A     | 530  | LYS  | N-CA-C      | 7.39  | 122.41      | 112.88   |
| 1   | A     | 1183 | GLY  | N-CA-C      | -7.39 | 102.97      | 115.08   |
| 1   | A     | 442  | GLU  | N-CA-C      | 7.28  | 126.31      | 110.80   |
| 1   | E     | 553  | HIS  | N-CA-C      | 7.13  | 125.99      | 110.80   |
| 1   | E     | 530  | LYS  | N-CA-C      | 7.05  | 122.89      | 113.72   |
| 1   | A     | 393  | GLU  | N-CA-C      | -6.66 | 103.49      | 111.69   |
| 1   | A     | 431  | LYS  | N-CA-C      | -6.65 | 98.99       | 109.50   |
| 1   | A     | 383  | ILE  | N-CA-C      | -6.47 | 97.64       | 107.73   |
| 1   | E     | 1165 | GLY  | N-CA-C      | 6.43  | 120.14      | 111.20   |
| 1   | A     | 715  | ILE  | N-CA-C      | 6.17  | 116.81      | 110.82   |
| 3   | G     | 309  | DA   | C2'-C3'-O3' | -6.13 | 102.30      | 111.50   |
| 1   | A     | 340  | VAL  | N-CA-C      | 6.12  | 116.32      | 107.88   |
| 1   | E     | 410  | MET  | N-CA-C      | -6.07 | 104.66      | 111.28   |
| 1   | E     | 800  | ASN  | N-CA-C      | 6.05  | 119.98      | 112.24   |
| 1   | A     | 552  | ASN  | CA-C-N      | 5.89  | 132.79      | 121.54   |
| 1   | A     | 552  | ASN  | C-N-CA      | 5.89  | 132.79      | 121.54   |
| 1   | E     | 340  | VAL  | N-CA-C      | 5.89  | 116.84      | 108.42   |
| 1   | A     | 535  | PRO  | CA-C-N      | -5.86 | 113.66      | 119.99   |
| 1   | A     | 535  | PRO  | C-N-CA      | -5.86 | 113.66      | 119.99   |
| 2   | B     | 8    | G    | C4'-C3'-O3' | 5.85  | 118.17      | 109.40   |
| 1   | E     | 1128 | VAL  | CA-C-N      | 5.84  | 126.18      | 119.93   |
| 1   | E     | 1128 | VAL  | C-N-CA      | 5.84  | 126.18      | 119.93   |
| 1   | A     | 1165 | GLY  | N-CA-C      | 5.76  | 119.20      | 111.20   |
| 1   | A     | 1242 | ASP  | CA-C-N      | 5.55  | 126.78      | 119.84   |
| 1   | A     | 1242 | ASP  | C-N-CA      | 5.55  | 126.78      | 119.84   |
| 1   | A     | 728  | ILE  | N-CA-C      | 5.53  | 115.67      | 110.30   |
| 1   | E     | 421  | ILE  | N-CA-C      | 5.36  | 116.43      | 111.45   |
| 2   | F     | 208  | G    | N9-C1'-C2'  | 5.34  | 122.01      | 114.00   |
| 1   | E     | 715  | ILE  | N-CA-C      | 5.32  | 116.09      | 110.72   |
| 1   | A     | 382  | ASN  | N-CA-C      | 5.30  | 118.89      | 111.74   |
| 1   | E     | 529  | ILE  | N-CA-C      | -5.27 | 100.74      | 108.11   |
| 1   | A     | 915  | ILE  | N-CA-C      | -5.25 | 105.42      | 110.72   |
| 1   | A     | 533  | SER  | N-CA-C      | 5.21  | 117.27      | 110.08   |
| 2   | B     | 8    | G    | C5'-C4'-C3' | -5.21 | 107.38      | 115.20   |
| 1   | A     | 800  | ASN  | N-CA-C      | 5.11  | 118.78      | 112.24   |
| 1   | E     | 994  | MET  | N-CA-C      | -5.08 | 106.93      | 112.72   |
| 1   | A     | 1069 | VAL  | N-CA-C      | -5.07 | 102.09      | 109.29   |
| 1   | E     | 508  | ASN  | N-CA-C      | -5.07 | 104.83      | 111.02   |
| 1   | E     | 776  | MET  | N-CA-C      | 5.03  | 117.49      | 111.71   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 658 | HIS  | N-CA-C | 5.00 | 117.27      | 111.02   |
| 1   | A     | 714 | GLN  | N-CA-C | 5.00 | 116.42      | 111.07   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | G     | 320 | DG   | Sidechain |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6947  | 0        | 7092     | 283     | 0            |
| 1   | E     | 6947  | 0        | 7092     | 318     | 0            |
| 2   | B     | 232   | 0        | 120      | 9       | 0            |
| 2   | F     | 232   | 0        | 120      | 6       | 0            |
| 3   | C     | 264   | 0        | 146      | 15      | 0            |
| 3   | G     | 264   | 0        | 146      | 15      | 0            |
| 4   | A     | 24    | 0        | 34       | 8       | 0            |
| 4   | E     | 24    | 0        | 34       | 6       | 0            |
| 5   | A     | 80    | 0        | 0        | 12      | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 3     | 0        | 0        | 2       | 0            |
| 5   | E     | 62    | 0        | 0        | 7       | 0            |
| 5   | F     | 3     | 0        | 0        | 0       | 0            |
| 5   | G     | 2     | 0        | 0        | 2       | 0            |
| All | All   | 15085 | 0        | 14784    | 647     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (647) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:908:MET:HE2 | 1:E:916:ARG:HH11 | 1.01                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:315:DT:H2''   | 3:G:316:DC:H5''   | 1.30                     | 1.14              |
| 1:E:394:MET:HE3   | 1:E:405:GLY:HA2   | 1.34                     | 1.09              |
| 1:A:652:ASN:HD22  | 1:A:670:MET:HE3   | 1.16                     | 1.06              |
| 1:A:1233:VAL:HG13 | 1:A:1243:PRO:HB3  | 1.36                     | 1.03              |
| 1:E:555:ASN:H     | 1:E:555:ASN:HD22  | 1.08                     | 1.01              |
| 1:A:1224:CYS:HA   | 1:A:1227:ILE:HD13 | 1.41                     | 1.00              |
| 1:A:908:MET:HE1   | 1:A:916:ARG:HD2   | 1.42                     | 1.00              |
| 4:A:1301:2ZE:H14  | 4:A:1301:2ZE:H4   | 1.41                     | 0.99              |
| 1:E:708:LEU:O     | 1:E:712:VAL:HG23  | 1.66                     | 0.96              |
| 3:G:315:DT:H2''   | 3:G:316:DC:C5'    | 1.96                     | 0.96              |
| 4:E:1301:2ZE:H14  | 4:E:1301:2ZE:H4   | 1.46                     | 0.95              |
| 3:C:120:DG:N7     | 5:C:201:HOH:O     | 1.99                     | 0.94              |
| 1:E:922:ARG:HG3   | 1:E:946:GLN:HE21  | 1.32                     | 0.94              |
| 1:E:410:MET:HE3   | 1:E:451:GLU:HG2   | 1.48                     | 0.94              |
| 1:E:1150:LYS:H    | 1:E:1150:LYS:HD2  | 1.31                     | 0.93              |
| 1:E:554:GLN:NE2   | 1:E:650:ARG:HH12  | 1.68                     | 0.92              |
| 1:E:727:ASN:N     | 1:E:727:ASN:HD22  | 1.67                     | 0.91              |
| 1:E:922:ARG:HG3   | 1:E:946:GLN:NE2   | 1.86                     | 0.90              |
| 1:A:908:MET:HE3   | 1:A:913:ARG:HG3   | 1.54                     | 0.90              |
| 1:A:1150:LYS:HD2  | 1:A:1150:LYS:H    | 1.37                     | 0.89              |
| 1:A:458:SER:HB3   | 1:A:461:MET:HE3   | 1.53                     | 0.89              |
| 1:A:354:ASN:HD22  | 1:A:354:ASN:N     | 1.69                     | 0.89              |
| 1:E:908:MET:HE2   | 1:E:916:ARG:NH1   | 1.87                     | 0.88              |
| 1:E:1040:ILE:N    | 5:E:1447:HOH:O    | 1.97                     | 0.86              |
| 1:E:555:ASN:H     | 1:E:555:ASN:ND2   | 1.73                     | 0.85              |
| 3:C:113:DG:OP2    | 5:C:202:HOH:O     | 1.93                     | 0.85              |
| 1:E:854:LYS:HG3   | 1:E:1011:ASN:HD22 | 1.41                     | 0.84              |
| 1:E:908:MET:CE    | 1:E:916:ARG:HH11  | 1.88                     | 0.83              |
| 1:E:1010:THR:HG22 | 1:E:1021:LEU:HD23 | 1.58                     | 0.83              |
| 1:E:346:LEU:HB3   | 1:E:689:MET:HE3   | 1.60                     | 0.83              |
| 1:A:727:ASN:HD22  | 1:A:727:ASN:N     | 1.74                     | 0.83              |
| 1:A:921:ARG:HD3   | 5:A:1479:HOH:O    | 1.79                     | 0.82              |
| 1:A:727:ASN:HD22  | 1:A:727:ASN:H     | 1.24                     | 0.82              |
| 1:E:840:ALA:HB3   | 5:E:1453:HOH:O    | 1.78                     | 0.81              |
| 1:A:1122:ASN:HA   | 1:A:1125:ASN:HD21 | 1.46                     | 0.80              |
| 1:E:727:ASN:HD22  | 1:E:727:ASN:H     | 1.29                     | 0.80              |
| 3:C:118:DA:H2''   | 3:C:119:DG:H5'    | 1.62                     | 0.79              |
| 1:A:791:LEU:HD23  | 1:A:956:MET:HE1   | 1.65                     | 0.79              |
| 1:E:785:SER:HB3   | 5:G:402:HOH:O     | 1.83                     | 0.79              |
| 1:A:555:ASN:HD22  | 1:A:555:ASN:H     | 1.27                     | 0.79              |
| 1:E:354:ASN:N     | 1:E:354:ASN:HD22  | 1.78                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1122:ASN:HA   | 1:E:1125:ASN:HD21 | 1.49                     | 0.78              |
| 3:C:115:DT:H2''   | 3:C:116:DC:C5'    | 2.14                     | 0.78              |
| 1:E:727:ASN:H     | 1:E:727:ASN:ND2   | 1.80                     | 0.77              |
| 1:A:1010:THR:HG22 | 1:A:1021:LEU:HD23 | 1.66                     | 0.77              |
| 1:A:636:GLY:HA3   | 1:A:639:ILE:HD11  | 1.65                     | 0.77              |
| 1:E:458:SER:HB3   | 1:E:461:MET:HE2   | 1.67                     | 0.76              |
| 1:E:672:LYS:HG3   | 1:E:673:LEU:H     | 1.50                     | 0.75              |
| 1:A:555:ASN:H     | 1:A:555:ASN:ND2   | 1.85                     | 0.75              |
| 1:A:365:VAL:HG22  | 1:A:376:CYS:HB2   | 1.69                     | 0.74              |
| 1:E:860:ASP:HB2   | 1:E:1041:ASP:HB2  | 1.69                     | 0.74              |
| 1:A:908:MET:CE    | 1:A:916:ARG:HD2   | 2.15                     | 0.74              |
| 1:A:1185:ASN:C    | 1:A:1185:ASN:HD22 | 1.94                     | 0.74              |
| 1:E:1233:VAL:HG13 | 1:E:1243:PRO:HB3  | 1.68                     | 0.74              |
| 1:E:554:GLN:HE22  | 1:E:650:ARG:HH12  | 1.34                     | 0.74              |
| 1:A:1234:LEU:HG   | 1:A:1238:TRP:CZ2  | 2.22                     | 0.73              |
| 3:C:115:DT:H2''   | 3:C:116:DC:H5'    | 1.69                     | 0.72              |
| 1:A:1212:LEU:HD23 | 1:A:1216:ILE:HD12 | 1.70                     | 0.72              |
| 1:E:908:MET:HE2   | 1:E:916:ARG:HD3   | 1.70                     | 0.72              |
| 1:E:340:VAL:HG23  | 1:E:501:VAL:O     | 1.88                     | 0.72              |
| 1:A:547:MET:HE1   | 1:A:589:PRO:HG3   | 1.70                     | 0.72              |
| 1:E:783:GLY:HA2   | 3:G:310:DG:OP2    | 1.90                     | 0.71              |
| 1:A:1095:VAL:O    | 1:A:1099:ILE:HG13 | 1.91                     | 0.71              |
| 1:E:1113:GLN:HG3  | 1:E:1238:TRP:NE1  | 2.05                     | 0.71              |
| 1:E:875:CYS:HB2   | 1:E:912:PRO:HD3   | 1.73                     | 0.70              |
| 1:A:397:ASP:OD2   | 1:A:400:THR:HG23  | 1.90                     | 0.70              |
| 3:C:120:DG:H2''   | 3:C:121:DC:OP2    | 1.92                     | 0.70              |
| 2:F:208:G:H1'     | 2:F:209:C:C6      | 2.26                     | 0.70              |
| 1:E:529:ILE:HD11  | 1:E:532:VAL:HG23  | 1.72                     | 0.70              |
| 1:E:730:ASN:N     | 1:E:730:ASN:HD22  | 1.90                     | 0.70              |
| 1:E:636:GLY:HA3   | 1:E:639:ILE:HD11  | 1.74                     | 0.69              |
| 1:E:1150:LYS:HD2  | 1:E:1150:LYS:N    | 2.06                     | 0.69              |
| 1:A:1225:GLU:HB3  | 1:A:1226:PRO:HD3  | 1.73                     | 0.69              |
| 1:E:667:ARG:NH1   | 1:E:683:ASN:O     | 2.25                     | 0.69              |
| 1:A:544:MET:HE2   | 1:A:560:MET:HE3   | 1.75                     | 0.69              |
| 1:A:727:ASN:H     | 1:A:727:ASN:ND2   | 1.91                     | 0.68              |
| 1:E:915:ILE:HD11  | 1:E:956:MET:HG2   | 1.75                     | 0.68              |
| 1:E:1113:GLN:HG3  | 1:E:1238:TRP:CE2  | 2.29                     | 0.68              |
| 1:A:652:ASN:ND2   | 1:A:670:MET:HE3   | 2.00                     | 0.68              |
| 1:A:1104:SER:HA   | 5:A:1473:HOH:O    | 1.93                     | 0.68              |
| 3:C:109:DA:H4'    | 3:C:110:DG:OP2    | 1.93                     | 0.68              |
| 1:A:1224:CYS:CA   | 1:A:1227:ILE:HD13 | 2.20                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:863:SER:HA    | 5:A:1411:HOH:O    | 1.95                     | 0.67              |
| 1:E:730:ASN:H     | 1:E:730:ASN:ND2   | 1.92                     | 0.67              |
| 1:E:1225:GLU:HB3  | 1:E:1226:PRO:HD3  | 1.76                     | 0.67              |
| 1:E:854:LYS:HG3   | 1:E:1011:ASN:HA   | 1.76                     | 0.67              |
| 1:E:1122:ASN:HA   | 1:E:1125:ASN:ND2  | 2.09                     | 0.67              |
| 1:A:667:ARG:NH1   | 1:A:683:ASN:O     | 2.27                     | 0.66              |
| 1:E:909:GLY:C     | 1:E:912:PRO:HD2   | 2.21                     | 0.66              |
| 1:E:865:TYR:HB2   | 1:E:866:PRO:HD3   | 1.77                     | 0.66              |
| 3:G:318:DA:H2''   | 3:G:319:DG:H5'    | 1.77                     | 0.66              |
| 2:B:10:G:H2'      | 2:B:11:DC:C6      | 2.31                     | 0.66              |
| 1:A:1105:ARG:O    | 1:A:1109:VAL:HG23 | 1.96                     | 0.65              |
| 1:E:935:ASN:HB3   | 1:E:938:LEU:HD22  | 1.78                     | 0.65              |
| 1:E:595:PRO:HD3   | 1:E:732:TYR:O     | 1.97                     | 0.65              |
| 1:A:1217:HIS:HB3  | 1:A:1218:PRO:HD3  | 1.79                     | 0.65              |
| 1:E:1115:ARG:O    | 1:E:1119:ILE:HG12 | 1.96                     | 0.65              |
| 1:A:618:LEU:HD23  | 1:A:619:LEU:N     | 2.12                     | 0.65              |
| 1:E:1211:TYR:O    | 1:E:1216:ILE:HG13 | 1.96                     | 0.65              |
| 1:E:408:ILE:HD13  | 1:E:472:THR:HA    | 1.79                     | 0.65              |
| 4:A:1301:2ZE:H4   | 4:A:1301:2ZE:CAS  | 2.24                     | 0.65              |
| 1:E:652:ASN:HD22  | 1:E:670:MET:CE    | 2.09                     | 0.65              |
| 1:E:1026:LYS:HG3  | 1:E:1030:ASN:ND2  | 2.11                     | 0.64              |
| 1:E:1109:VAL:HG13 | 1:E:1230:ILE:CD1  | 2.27                     | 0.64              |
| 1:A:352:GLN:HB2   | 5:A:1438:HOH:O    | 1.98                     | 0.64              |
| 1:A:1109:VAL:HG13 | 1:A:1230:ILE:CD1  | 2.28                     | 0.64              |
| 1:A:1149:LYS:HG2  | 1:A:1150:LYS:N    | 2.11                     | 0.64              |
| 1:A:860:ASP:HB2   | 1:A:1041:ASP:HB2  | 1.79                     | 0.63              |
| 1:E:669:ASN:HD22  | 1:E:669:ASN:N     | 1.95                     | 0.63              |
| 1:A:962:PHE:CZ    | 3:C:109:DA:H5'    | 2.34                     | 0.63              |
| 1:A:595:PRO:HG3   | 1:A:732:TYR:O     | 1.99                     | 0.62              |
| 1:E:1185:ASN:HD22 | 1:E:1185:ASN:C    | 2.08                     | 0.62              |
| 1:A:555:ASN:HD22  | 1:A:555:ASN:N     | 1.94                     | 0.62              |
| 1:A:962:PHE:HZ    | 3:C:109:DA:H5'    | 1.64                     | 0.62              |
| 1:E:725:MET:SD    | 1:E:1166:GLY:HA3  | 2.39                     | 0.62              |
| 1:A:806:LYS:HD2   | 5:A:1480:HOH:O    | 1.99                     | 0.62              |
| 4:A:1301:2ZE:H14  | 4:A:1301:2ZE:CAW  | 2.25                     | 0.62              |
| 3:C:115:DT:H2''   | 3:C:116:DC:H5''   | 1.81                     | 0.62              |
| 1:E:507:LEU:HD12  | 1:E:507:LEU:N     | 2.15                     | 0.62              |
| 1:E:730:ASN:N     | 1:E:730:ASN:ND2   | 2.47                     | 0.62              |
| 1:A:354:ASN:N     | 1:A:354:ASN:ND2   | 2.43                     | 0.61              |
| 1:A:1111:ASN:N    | 1:A:1111:ASN:HD22 | 1.96                     | 0.61              |
| 1:E:354:ASN:N     | 1:E:354:ASN:ND2   | 2.47                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1181:GLN:HB2  | 1:A:1205:THR:HG23 | 1.83                     | 0.61              |
| 2:B:8:G:H1'       | 2:B:9:C:C6        | 2.36                     | 0.61              |
| 1:E:857:LEU:HD11  | 1:E:1022:GLY:CA   | 2.31                     | 0.61              |
| 1:E:1113:GLN:HE21 | 1:E:1238:TRP:HE1  | 1.49                     | 0.61              |
| 4:E:1301:2ZE:H4   | 4:E:1301:2ZE:CAS  | 2.27                     | 0.61              |
| 1:A:926:LYS:HE3   | 1:A:946:GLN:HG3   | 1.83                     | 0.61              |
| 1:E:436:GLU:O     | 1:E:437:LYS:HG2   | 2.00                     | 0.61              |
| 1:A:1216:ILE:O    | 1:A:1220:VAL:HG23 | 2.01                     | 0.61              |
| 1:E:785:SER:CB    | 5:G:402:HOH:O     | 2.47                     | 0.61              |
| 1:E:555:ASN:ND2   | 1:E:555:ASN:N     | 2.39                     | 0.60              |
| 1:E:1047:LEU:HD12 | 1:E:1048:LEU:N    | 2.16                     | 0.60              |
| 1:A:570:LEU:HD22  | 1:A:762:LEU:HB3   | 1.83                     | 0.60              |
| 1:A:788:ASN:ND2   | 1:A:959:CYS:HB3   | 2.16                     | 0.60              |
| 1:A:1122:ASN:HA   | 1:A:1125:ASN:ND2  | 2.13                     | 0.60              |
| 1:E:444:PRO:O     | 1:E:445:ASP:HB2   | 2.00                     | 0.60              |
| 1:A:1231:ASP:OD2  | 1:A:1234:LEU:HB2  | 2.01                     | 0.60              |
| 1:A:898:ILE:N     | 1:A:898:ILE:HD13  | 2.17                     | 0.60              |
| 1:E:410:MET:HG2   | 1:E:434:PRO:HB3   | 1.82                     | 0.60              |
| 1:E:365:VAL:HG22  | 1:E:376:CYS:HB2   | 1.81                     | 0.60              |
| 1:A:911:LEU:HD11  | 1:A:956:MET:HG2   | 1.84                     | 0.60              |
| 1:E:672:LYS:NZ    | 1:E:672:LYS:HB2   | 2.17                     | 0.59              |
| 1:E:792:LEU:HD21  | 1:E:956:MET:CE    | 2.32                     | 0.59              |
| 1:E:1230:ILE:HA   | 1:E:1234:LEU:HD23 | 1.84                     | 0.59              |
| 1:A:682:ARG:O     | 1:A:682:ARG:HD3   | 2.03                     | 0.59              |
| 1:E:597:ALA:O     | 1:E:601:VAL:HG23  | 2.03                     | 0.59              |
| 1:E:849:VAL:HG13  | 1:E:1049:LEU:O    | 2.03                     | 0.59              |
| 1:E:935:ASN:HD22  | 1:E:935:ASN:C     | 2.09                     | 0.59              |
| 1:E:1010:THR:HG22 | 1:E:1021:LEU:CD2  | 2.29                     | 0.59              |
| 1:A:1148:ASP:OD1  | 1:A:1151:SER:HB3  | 2.03                     | 0.58              |
| 1:E:398:LEU:O     | 1:E:399:ASN:HB2   | 2.02                     | 0.58              |
| 1:E:1170:LYS:O    | 1:E:1173:ASP:HB2  | 2.03                     | 0.58              |
| 1:A:555:ASN:ND2   | 1:A:555:ASN:N     | 2.48                     | 0.58              |
| 1:E:588:LYS:HD3   | 1:E:594:PHE:CE1   | 2.37                     | 0.58              |
| 1:A:935:ASN:ND2   | 1:A:937:ASP:OD1   | 2.34                     | 0.58              |
| 1:E:438:ASN:HA    | 1:E:448:GLU:O     | 2.02                     | 0.58              |
| 1:E:607:VAL:HB    | 1:E:609:VAL:HG12  | 1.85                     | 0.58              |
| 1:E:760:ASN:O     | 1:E:763:PRO:HD2   | 2.04                     | 0.58              |
| 1:E:963:SER:HA    | 1:E:968:TYR:CE1   | 2.38                     | 0.58              |
| 1:E:1227:ILE:N    | 1:E:1227:ILE:HD12 | 2.18                     | 0.58              |
| 1:A:1048:LEU:HG   | 1:A:1050:LEU:HD21 | 1.85                     | 0.58              |
| 1:E:1109:VAL:HG13 | 1:E:1230:ILE:HD11 | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:369:SER:HB3   | 5:A:1424:HOH:O    | 2.03                     | 0.58              |
| 1:E:540:MET:HE1   | 1:E:626:VAL:HG22  | 1.86                     | 0.58              |
| 1:E:908:MET:HE3   | 1:E:913:ARG:HA    | 1.86                     | 0.57              |
| 1:E:586:VAL:HB    | 1:E:742:LEU:HD21  | 1.86                     | 0.57              |
| 1:E:644:LEU:HD23  | 1:E:681:GLU:HB3   | 1.86                     | 0.57              |
| 1:E:1224:CYS:HA   | 1:E:1227:ILE:HD13 | 1.86                     | 0.57              |
| 2:F:201:G:H2'     | 2:F:202:C:C6      | 2.39                     | 0.57              |
| 1:E:555:ASN:HD22  | 1:E:555:ASN:N     | 1.80                     | 0.57              |
| 1:E:668:SER:C     | 1:E:669:ASN:HD22  | 2.13                     | 0.57              |
| 1:A:1233:VAL:CG1  | 1:A:1243:PRO:HB3  | 2.22                     | 0.57              |
| 1:E:727:ASN:N     | 1:E:727:ASN:ND2   | 2.35                     | 0.57              |
| 1:A:774:ASN:HB2   | 5:A:1433:HOH:O    | 2.04                     | 0.56              |
| 1:A:704:LYS:HD2   | 1:A:1136:ASN:ND2  | 2.19                     | 0.56              |
| 1:E:788:ASN:ND2   | 1:E:959:CYS:HB3   | 2.19                     | 0.56              |
| 1:A:1010:THR:HG22 | 1:A:1021:LEU:CD2  | 2.34                     | 0.56              |
| 1:E:382:ASN:ND2   | 1:E:521:LEU:O     | 2.34                     | 0.56              |
| 1:A:538:VAL:CG1   | 1:A:631:PRO:HA    | 2.36                     | 0.56              |
| 1:E:554:GLN:NE2   | 1:E:650:ARG:NH1   | 2.48                     | 0.56              |
| 1:A:346:LEU:HB3   | 1:A:689:MET:HE2   | 1.88                     | 0.56              |
| 1:A:410:MET:CE    | 1:A:451:GLU:HG2   | 2.35                     | 0.56              |
| 1:E:652:ASN:HD22  | 1:E:670:MET:HE2   | 1.69                     | 0.56              |
| 1:E:900:GLU:HG3   | 5:E:1441:HOH:O    | 2.03                     | 0.56              |
| 1:E:1217:HIS:HB3  | 1:E:1218:PRO:HD3  | 1.85                     | 0.56              |
| 1:E:570:LEU:HD22  | 1:E:762:LEU:HB3   | 1.88                     | 0.56              |
| 1:A:1047:LEU:HD12 | 1:A:1048:LEU:N    | 2.21                     | 0.56              |
| 4:E:1301:2ZE:H14  | 4:E:1301:2ZE:CAW  | 2.29                     | 0.56              |
| 1:E:1154:HIS:CE1  | 1:E:1155:VAL:HG23 | 2.41                     | 0.56              |
| 1:E:618:LEU:C     | 1:E:618:LEU:HD23  | 2.30                     | 0.56              |
| 1:A:875:CYS:HB2   | 1:A:912:PRO:HD3   | 1.87                     | 0.55              |
| 1:A:395:LYS:HB2   | 1:A:408:ILE:HD11  | 1.88                     | 0.55              |
| 1:A:410:MET:HE3   | 1:A:451:GLU:HG2   | 1.88                     | 0.55              |
| 1:A:411:LYS:HE2   | 1:A:415:GLU:OE2   | 2.06                     | 0.55              |
| 1:E:408:ILE:HG23  | 1:E:412:ASP:HB2   | 1.89                     | 0.55              |
| 3:G:311:DG:H2''   | 3:G:312:DC:H5'    | 1.88                     | 0.55              |
| 1:A:538:VAL:HG12  | 1:A:631:PRO:HA    | 1.87                     | 0.55              |
| 1:A:970:LYS:HB3   | 1:A:971:PRO:HD3   | 1.89                     | 0.55              |
| 1:E:399:ASN:O     | 1:E:400:THR:C     | 2.50                     | 0.55              |
| 1:E:1212:LEU:HD23 | 1:E:1216:ILE:HD12 | 1.87                     | 0.55              |
| 1:E:1058:LEU:HB3  | 1:E:1070:THR:OG1  | 2.07                     | 0.55              |
| 1:E:1095:VAL:O    | 1:E:1099:ILE:HG13 | 2.07                     | 0.55              |
| 1:A:652:ASN:HD22  | 1:A:670:MET:CE    | 2.04                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1231:ASP:O    | 1:A:1235:ILE:HG13 | 2.06                     | 0.55              |
| 1:E:500:GLU:OE2   | 1:E:502:LYS:HE3   | 2.06                     | 0.55              |
| 1:E:1002:ASP:O    | 1:E:1004:ASP:N    | 2.35                     | 0.55              |
| 1:A:708:LEU:O     | 1:A:712:VAL:HG23  | 2.07                     | 0.55              |
| 1:E:1149:LYS:HE3  | 1:E:1159:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:394:MET:HG2   | 1:A:403:GLU:OE1   | 2.06                     | 0.54              |
| 1:E:1119:ILE:O    | 1:E:1123:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:1227:ILE:HD12 | 1:A:1227:ILE:N    | 2.23                     | 0.54              |
| 1:E:432:SER:HA    | 1:E:454:GLU:O     | 2.07                     | 0.54              |
| 1:E:669:ASN:N     | 1:E:669:ASN:ND2   | 2.55                     | 0.54              |
| 1:A:1026:LYS:HG2  | 1:A:1027:SER:N    | 2.22                     | 0.54              |
| 1:A:1082:ARG:HG2  | 1:A:1136:ASN:O    | 2.08                     | 0.54              |
| 1:E:1113:GLN:O    | 1:E:1117:ILE:HG13 | 2.08                     | 0.54              |
| 1:E:652:ASN:ND2   | 1:E:670:MET:HE2   | 2.23                     | 0.54              |
| 1:E:903:ASP:OD2   | 1:E:905:SER:HB3   | 2.08                     | 0.54              |
| 1:A:1184:SER:O    | 1:A:1185:ASN:ND2  | 2.40                     | 0.53              |
| 1:E:627:HIS:HB2   | 1:E:661:LYS:HD3   | 1.90                     | 0.53              |
| 1:A:1095:VAL:HG13 | 1:A:1112:ILE:HD13 | 1.90                     | 0.53              |
| 1:A:1211:TYR:O    | 1:A:1215:GLN:HB2  | 2.09                     | 0.53              |
| 1:E:788:ASN:CB    | 1:E:959:CYS:SG    | 2.97                     | 0.53              |
| 1:E:911:LEU:HB3   | 1:E:912:PRO:HD3   | 1.91                     | 0.53              |
| 1:A:442:GLU:HB2   | 5:A:1463:HOH:O    | 2.07                     | 0.53              |
| 2:B:8:G:HO2'      | 2:B:9:C:H5        | 1.54                     | 0.53              |
| 1:E:564:VAL:HG21  | 1:E:629:ILE:HD13  | 1.91                     | 0.53              |
| 1:A:437:LYS:HB3   | 1:A:802:ILE:HG12  | 1.91                     | 0.53              |
| 1:A:1002:ASP:O    | 1:A:1004:ASP:N    | 2.39                     | 0.53              |
| 1:E:1084:TRP:O    | 1:E:1089:LYS:HE2  | 2.09                     | 0.53              |
| 1:A:873:ASN:HD21  | 1:A:878:THR:HG21  | 1.74                     | 0.53              |
| 1:E:353:TYR:HD2   | 1:E:354:ASN:ND2   | 2.07                     | 0.53              |
| 1:E:544:MET:HE2   | 1:E:560:MET:HE3   | 1.91                     | 0.53              |
| 1:E:792:LEU:HD21  | 1:E:956:MET:HE2   | 1.90                     | 0.53              |
| 1:A:909:GLY:C     | 1:A:912:PRO:HD2   | 2.33                     | 0.53              |
| 3:G:315:DT:C2'    | 3:G:316:DC:H5''   | 2.21                     | 0.53              |
| 1:A:1064:SER:O    | 1:A:1067:ASN:HB2  | 2.08                     | 0.52              |
| 1:A:1109:VAL:HG13 | 1:A:1230:ILE:HD11 | 1.91                     | 0.52              |
| 1:E:854:LYS:HG3   | 1:E:1011:ASN:ND2  | 2.18                     | 0.52              |
| 1:E:476:VAL:HG12  | 5:E:1436:HOH:O    | 2.08                     | 0.52              |
| 1:E:523:PRO:C     | 1:E:525:LEU:H     | 2.18                     | 0.52              |
| 1:E:728:ILE:HG22  | 1:E:729:GLN:N     | 2.23                     | 0.52              |
| 1:A:432:SER:HA    | 1:A:454:GLU:O     | 2.09                     | 0.52              |
| 1:A:935:ASN:HD22  | 1:A:936:PRO:HD2   | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:365:VAL:HA    | 5:E:1404:HOH:O    | 2.08                     | 0.52              |
| 1:E:1026:LYS:HG3  | 1:E:1030:ASN:HD21 | 1.73                     | 0.52              |
| 1:E:1241:LEU:O    | 1:E:1243:PRO:HD3  | 2.08                     | 0.52              |
| 1:A:428:MET:SD    | 1:A:428:MET:N     | 2.83                     | 0.52              |
| 1:A:537:LEU:HD12  | 1:A:633:ILE:HD11  | 1.92                     | 0.52              |
| 1:A:855:PHE:HD2   | 1:A:1018:VAL:HG21 | 1.75                     | 0.52              |
| 1:A:1084:TRP:O    | 1:A:1089:LYS:HE2  | 2.10                     | 0.52              |
| 1:A:618:LEU:HD23  | 1:A:618:LEU:C     | 2.35                     | 0.52              |
| 1:E:1138:ALA:HA   | 1:E:1174:THR:HA   | 1.92                     | 0.52              |
| 1:A:1241:LEU:O    | 1:A:1243:PRO:HD3  | 2.10                     | 0.52              |
| 1:A:913:ARG:HD2   | 5:A:1442:HOH:O    | 2.09                     | 0.52              |
| 1:A:1113:GLN:HE21 | 1:A:1238:TRP:NE1  | 2.07                     | 0.52              |
| 1:E:1215:GLN:C    | 1:E:1218:PRO:HD2  | 2.35                     | 0.51              |
| 1:A:425:TYR:C     | 1:A:426:LYS:HG2   | 2.36                     | 0.51              |
| 1:A:529:ILE:HD12  | 1:E:342:HIS:CE1   | 2.45                     | 0.51              |
| 1:A:1111:ASN:N    | 1:A:1111:ASN:ND2  | 2.57                     | 0.51              |
| 1:E:1020:LYS:O    | 1:E:1024:LYS:HB2  | 2.10                     | 0.51              |
| 1:E:1198:LEU:HG   | 1:E:1199:GLN:N    | 2.25                     | 0.51              |
| 1:A:727:ASN:O     | 1:A:731:MET:HG3   | 2.10                     | 0.51              |
| 1:A:1010:THR:C    | 1:A:1012:SER:H    | 2.18                     | 0.51              |
| 1:A:1116:LEU:CD2  | 1:A:1235:ILE:HG23 | 2.40                     | 0.51              |
| 1:A:1150:LYS:HD2  | 1:A:1150:LYS:N    | 2.15                     | 0.51              |
| 1:A:728:ILE:HG22  | 1:A:729:GLN:N     | 2.24                     | 0.51              |
| 1:A:1196:GLU:HG3  | 1:A:1197:GLN:N    | 2.26                     | 0.51              |
| 1:E:340:VAL:HG21  | 1:E:500:GLU:CG    | 2.41                     | 0.51              |
| 1:A:854:LYS:HG3   | 1:A:1011:ASN:HD22 | 1.75                     | 0.51              |
| 1:E:506:LEU:C     | 1:E:507:LEU:HD12  | 2.35                     | 0.51              |
| 1:E:391:PRO:HG3   | 1:E:410:MET:HE1   | 1.92                     | 0.51              |
| 1:E:843:LEU:HD21  | 1:E:985:MET:HE2   | 1.93                     | 0.51              |
| 1:E:1219:VAL:O    | 1:E:1223:ILE:HG13 | 2.10                     | 0.51              |
| 1:A:875:CYS:SG    | 1:A:876:PHE:N     | 2.84                     | 0.51              |
| 1:E:1148:ASP:CG   | 1:E:1148:ASP:O    | 2.54                     | 0.51              |
| 1:E:1109:VAL:HG13 | 1:E:1230:ILE:HD13 | 1.93                     | 0.51              |
| 1:E:704:LYS:HA    | 1:E:1082:ARG:HE   | 1.77                     | 0.50              |
| 1:E:762:LEU:HB2   | 1:E:763:PRO:HD3   | 1.93                     | 0.50              |
| 1:E:794:HIS:O     | 1:E:798:GLU:HG3   | 2.10                     | 0.50              |
| 1:E:370:ALA:O     | 1:E:372:THR:HG22  | 2.11                     | 0.50              |
| 1:E:394:MET:CE    | 1:E:405:GLY:HA2   | 2.25                     | 0.50              |
| 1:E:562:ALA:C     | 1:E:563:LEU:HD12  | 2.36                     | 0.50              |
| 1:A:588:LYS:O     | 1:A:589:PRO:O     | 2.29                     | 0.50              |
| 1:A:652:ASN:HB2   | 1:A:670:MET:CE    | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1113:GLN:O    | 1:A:1117:ILE:HG13 | 2.12                     | 0.50              |
| 1:A:1181:GLN:HA   | 1:A:1181:GLN:NE2  | 2.26                     | 0.50              |
| 1:A:1181:GLN:HA   | 1:A:1181:GLN:HE21 | 1.77                     | 0.50              |
| 1:A:682:ARG:HD3   | 1:A:682:ARG:C     | 2.36                     | 0.50              |
| 1:A:1069:VAL:HG12 | 1:A:1070:THR:H    | 1.77                     | 0.50              |
| 1:A:1210:TYR:CD1  | 1:A:1214:GLN:HG3  | 2.47                     | 0.50              |
| 2:F:202:C:H2'     | 2:F:203:C:C6      | 2.47                     | 0.50              |
| 1:A:563:LEU:HD22  | 1:A:750:LYS:HA    | 1.94                     | 0.50              |
| 1:A:1109:VAL:HG13 | 1:A:1230:ILE:HD13 | 1.93                     | 0.50              |
| 1:A:1219:VAL:O    | 1:A:1223:ILE:HG13 | 2.12                     | 0.50              |
| 1:A:986:HIS:CD2   | 1:A:986:HIS:O     | 2.65                     | 0.49              |
| 1:A:1030:ASN:OD1  | 1:A:1038:ILE:HG22 | 2.12                     | 0.49              |
| 4:A:1301:2ZE:H18  | 3:C:111:DG:C2     | 2.47                     | 0.49              |
| 1:E:672:LYS:CG    | 1:E:673:LEU:H     | 2.23                     | 0.49              |
| 1:E:858:LEU:C     | 1:E:858:LEU:HD12  | 2.37                     | 0.49              |
| 1:E:1095:VAL:HG13 | 1:E:1112:ILE:HD13 | 1.94                     | 0.49              |
| 1:E:1096:ILE:HD11 | 1:E:1223:ILE:HG23 | 1.93                     | 0.49              |
| 1:A:619:LEU:HD13  | 1:A:651:ILE:HA    | 1.94                     | 0.49              |
| 1:E:704:LYS:O     | 1:E:1174:THR:HG21 | 2.11                     | 0.49              |
| 1:A:854:LYS:HG3   | 1:A:1011:ASN:HA   | 1.94                     | 0.49              |
| 1:A:978:TYR:C     | 1:A:980:GLY:N     | 2.66                     | 0.49              |
| 1:E:340:VAL:HG22  | 1:E:341:PHE:N     | 2.27                     | 0.49              |
| 1:A:1056:ALA:HB2  | 1:A:1077:LEU:HD11 | 1.95                     | 0.49              |
| 1:E:870:GLN:HE22  | 1:E:919:VAL:HG21  | 1.76                     | 0.49              |
| 1:E:1112:ILE:O    | 1:E:1116:LEU:HD13 | 2.12                     | 0.49              |
| 1:A:669:ASN:N     | 1:A:669:ASN:HD22  | 2.10                     | 0.49              |
| 1:E:908:MET:O     | 1:E:913:ARG:NH1   | 2.44                     | 0.49              |
| 1:E:1074:LEU:O    | 1:E:1075:LYS:HG2  | 2.13                     | 0.49              |
| 1:A:788:ASN:ND2   | 1:A:959:CYS:CB    | 2.75                     | 0.49              |
| 1:E:837:ALA:HB1   | 3:G:312:DC:H3'    | 1.95                     | 0.49              |
| 1:A:1115:ARG:O    | 1:A:1119:ILE:HG12 | 2.13                     | 0.49              |
| 1:E:1030:ASN:OD1  | 1:E:1038:ILE:HG22 | 2.13                     | 0.49              |
| 1:A:644:LEU:HD23  | 1:A:681:GLU:HB3   | 1.94                     | 0.49              |
| 1:E:432:SER:HB2   | 1:E:453:LEU:HD11  | 1.93                     | 0.49              |
| 1:E:602:ILE:HG21  | 1:E:609:VAL:HG13  | 1.94                     | 0.49              |
| 1:A:865:TYR:HB2   | 1:A:866:PRO:HD3   | 1.95                     | 0.49              |
| 1:A:1116:LEU:HD22 | 1:A:1238:TRP:HE3  | 1.76                     | 0.49              |
| 1:E:529:ILE:C     | 1:E:529:ILE:HD12  | 2.38                     | 0.49              |
| 1:E:652:ASN:HD22  | 1:E:670:MET:HE3   | 1.77                     | 0.49              |
| 1:E:1105:ARG:O    | 1:E:1109:VAL:HG23 | 2.13                     | 0.49              |
| 3:G:320:DG:H2''   | 3:G:321:DC:OP2    | 2.11                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:834:ARG:NH2  | 3:C:112:DC:C5     | 2.81                     | 0.49              |
| 1:E:1148:ASP:OD1 | 1:E:1151:SER:HB3  | 2.12                     | 0.49              |
| 1:A:1215:GLN:C   | 1:A:1218:PRO:HD2  | 2.38                     | 0.48              |
| 1:E:385:ARG:HD2  | 1:E:457:TYR:CZ    | 2.47                     | 0.48              |
| 1:A:598:PHE:CZ   | 1:A:738:LEU:HD13  | 2.48                     | 0.48              |
| 1:A:875:CYS:HB2  | 1:A:912:PRO:CD    | 2.43                     | 0.48              |
| 1:A:807:GLN:HA   | 1:A:807:GLN:OE1   | 2.13                     | 0.48              |
| 1:E:963:SER:HA   | 1:E:968:TYR:CD1   | 2.48                     | 0.48              |
| 1:E:1053:LYS:O   | 1:E:1054:LYS:HG3  | 2.14                     | 0.48              |
| 2:F:201:G:H2'    | 2:F:202:C:H6      | 1.78                     | 0.48              |
| 1:E:672:LYS:HG3  | 1:E:673:LEU:N     | 2.22                     | 0.48              |
| 1:E:1021:LEU:O   | 1:E:1025:VAL:HG23 | 2.13                     | 0.48              |
| 2:B:5:G:O2'      | 2:B:6:G:H5'       | 2.14                     | 0.48              |
| 1:E:1079:ILE:O   | 1:E:1089:LYS:HD2  | 2.14                     | 0.48              |
| 1:A:541:ALA:HA   | 1:A:635:VAL:HG13  | 1.95                     | 0.48              |
| 1:A:760:ASN:O    | 1:A:763:PRO:HD2   | 2.13                     | 0.48              |
| 1:A:935:ASN:HD22 | 1:A:936:PRO:CD    | 2.26                     | 0.48              |
| 1:E:672:LYS:HB2  | 1:E:672:LYS:HZ3   | 1.77                     | 0.48              |
| 1:A:854:LYS:O    | 1:A:856:ILE:HD12  | 2.13                     | 0.48              |
| 1:E:846:ASP:OD1  | 1:E:847:PRO:HD2   | 2.14                     | 0.48              |
| 1:E:385:ARG:HD2  | 1:E:457:TYR:CE2   | 2.49                     | 0.48              |
| 1:E:1010:THR:CG2 | 1:E:1021:LEU:HD23 | 2.37                     | 0.48              |
| 1:A:586:VAL:HG22 | 1:A:587:SER:N     | 2.29                     | 0.47              |
| 1:A:785:SER:O    | 1:A:788:ASN:HB3   | 2.14                     | 0.47              |
| 1:E:858:LEU:HD12 | 1:E:859:LEU:N     | 2.28                     | 0.47              |
| 1:E:1162:ASN:OD1 | 1:E:1169:VAL:N    | 2.44                     | 0.47              |
| 1:A:550:ALA:O    | 1:A:551:LYS:O     | 2.32                     | 0.47              |
| 1:A:873:ASN:ND2  | 1:A:878:THR:HG21  | 2.28                     | 0.47              |
| 1:A:922:ARG:HE   | 1:A:946:GLN:HG2   | 1.79                     | 0.47              |
| 1:A:1211:TYR:O   | 1:A:1216:ILE:HG13 | 2.14                     | 0.47              |
| 1:E:429:LYS:HA   | 5:E:1428:HOH:O    | 2.13                     | 0.47              |
| 1:E:728:ILE:HA   | 1:E:731:MET:SD    | 2.54                     | 0.47              |
| 1:A:548:GLN:H    | 1:A:725:MET:CE    | 2.28                     | 0.47              |
| 1:A:423:THR:OG1  | 1:A:424:LYS:N     | 2.46                     | 0.47              |
| 1:E:548:GLN:HE21 | 1:E:548:GLN:HB2   | 1.45                     | 0.47              |
| 1:A:491:ARG:NH2  | 1:A:527:ASN:OD1   | 2.48                     | 0.47              |
| 1:A:664:ARG:HB2  | 1:A:687:GLY:HA3   | 1.95                     | 0.47              |
| 1:A:428:MET:C    | 1:A:429:LYS:HD2   | 2.39                     | 0.47              |
| 1:A:849:VAL:HG13 | 1:A:1049:LEU:O    | 2.14                     | 0.47              |
| 1:A:1079:ILE:CD1 | 1:A:1096:ILE:HG13 | 2.45                     | 0.47              |
| 1:E:1128:VAL:HB  | 1:E:1133:PHE:CZ   | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:652:ASN:HB2   | 1:A:670:MET:HE1   | 1.97                     | 0.47              |
| 1:A:903:ASP:OD2   | 1:A:905:SER:HB3   | 2.14                     | 0.47              |
| 1:A:1078:ASP:HB3  | 1:A:1084:TRP:CD1  | 2.50                     | 0.47              |
| 1:A:1105:ARG:NH2  | 1:A:1108:ILE:CD1  | 2.77                     | 0.47              |
| 1:E:935:ASN:O     | 1:E:938:LEU:HB2   | 2.13                     | 0.47              |
| 1:E:1227:ILE:N    | 1:E:1227:ILE:CD1  | 2.77                     | 0.47              |
| 1:E:728:ILE:O     | 1:E:731:MET:HB2   | 2.15                     | 0.47              |
| 1:A:927:GLN:NE2   | 1:A:930:LYS:HD2   | 2.30                     | 0.47              |
| 1:A:978:TYR:C     | 1:A:980:GLY:H     | 2.22                     | 0.47              |
| 1:A:1112:ILE:HG22 | 1:A:1116:LEU:HD13 | 1.97                     | 0.47              |
| 1:A:1134:GLU:HG2  | 1:A:1195:PRO:HG3  | 1.96                     | 0.47              |
| 1:E:529:ILE:HD11  | 1:E:532:VAL:CG2   | 2.43                     | 0.47              |
| 1:E:1216:ILE:O    | 1:E:1220:VAL:HG23 | 2.15                     | 0.46              |
| 3:G:315:DT:H2''   | 3:G:316:DC:H5'    | 1.90                     | 0.46              |
| 1:A:537:LEU:N     | 1:A:537:LEU:HD23  | 2.29                     | 0.46              |
| 1:A:558:ILE:C     | 1:A:558:ILE:HD12  | 2.40                     | 0.46              |
| 1:A:881:ARG:HG2   | 1:A:881:ARG:HH11  | 1.80                     | 0.46              |
| 1:E:404:THR:OG1   | 1:E:405:GLY:N     | 2.49                     | 0.46              |
| 1:E:873:ASN:ND2   | 1:E:878:THR:HG21  | 2.30                     | 0.46              |
| 1:A:395:LYS:HD2   | 5:A:1453:HOH:O    | 2.14                     | 0.46              |
| 1:A:523:PRO:C     | 1:A:525:LEU:H     | 2.24                     | 0.46              |
| 1:A:911:LEU:HB3   | 1:A:912:PRO:HD3   | 1.96                     | 0.46              |
| 1:A:990:MET:HE1   | 1:A:1032:LEU:HD11 | 1.97                     | 0.46              |
| 1:E:353:TYR:HD2   | 1:E:354:ASN:HD21  | 1.63                     | 0.46              |
| 1:E:563:LEU:HD23  | 1:E:579:PHE:CD1   | 2.50                     | 0.46              |
| 1:E:908:MET:HE3   | 1:E:913:ARG:HG3   | 1.98                     | 0.46              |
| 1:E:990:MET:HG2   | 1:E:994:MET:CE    | 2.45                     | 0.46              |
| 1:A:986:HIS:O     | 1:A:986:HIS:HD2   | 1.99                     | 0.46              |
| 2:B:2:C:H2'       | 2:B:3:C:C6        | 2.51                     | 0.46              |
| 1:A:433:LYS:HE3   | 1:A:435:VAL:CG1   | 2.45                     | 0.46              |
| 1:A:1152:LEU:HA   | 1:A:1153:PRO:HD2  | 1.81                     | 0.46              |
| 1:E:908:MET:CE    | 1:E:913:ARG:HA    | 2.46                     | 0.46              |
| 1:A:410:MET:HG2   | 1:A:434:PRO:HB3   | 1.97                     | 0.46              |
| 1:A:512:SER:HB2   | 1:A:664:ARG:O     | 2.15                     | 0.46              |
| 1:A:1010:THR:C    | 1:A:1012:SER:N    | 2.73                     | 0.46              |
| 1:E:875:CYS:SG    | 1:E:876:PHE:N     | 2.89                     | 0.46              |
| 1:E:931:GLN:HG2   | 1:E:932:GLN:N     | 2.29                     | 0.46              |
| 1:A:921:ARG:CD    | 5:A:1479:HOH:O    | 2.49                     | 0.46              |
| 1:A:928:LEU:O     | 1:A:931:GLN:HB2   | 2.16                     | 0.46              |
| 1:A:1050:LEU:N    | 1:A:1050:LEU:HD23 | 2.31                     | 0.46              |
| 1:E:531:ASP:OD1   | 1:E:531:ASP:N     | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:857:LEU:HD22  | 1:E:859:LEU:HD21  | 1.98                     | 0.46              |
| 1:A:1119:ILE:O    | 1:A:1123:VAL:HG23 | 2.15                     | 0.46              |
| 1:E:652:ASN:HB2   | 1:E:670:MET:CE    | 2.46                     | 0.46              |
| 1:A:500:GLU:HG2   | 5:A:1454:HOH:O    | 2.16                     | 0.46              |
| 1:A:932:GLN:NE2   | 1:A:932:GLN:HA    | 2.31                     | 0.46              |
| 1:E:340:VAL:HG23  | 1:E:501:VAL:C     | 2.41                     | 0.45              |
| 1:E:589:PRO:HG2   | 1:E:592:CYS:SG    | 2.56                     | 0.45              |
| 1:E:940:LEU:O     | 1:E:944:ILE:HD12  | 2.16                     | 0.45              |
| 1:A:602:ILE:HD13  | 1:A:609:VAL:HG13  | 1.97                     | 0.45              |
| 1:A:1055:TYR:CZ   | 1:A:1075:LYS:HG3  | 2.50                     | 0.45              |
| 1:E:938:LEU:HD12  | 1:E:938:LEU:HA    | 1.80                     | 0.45              |
| 1:A:705:SER:HA    | 1:A:1174:THR:HG21 | 1.98                     | 0.45              |
| 1:A:882:VAL:HG22  | 1:A:882:VAL:O     | 2.16                     | 0.45              |
| 1:E:783:GLY:CA    | 3:G:310:DG:OP2    | 2.64                     | 0.45              |
| 1:E:1148:ASP:O    | 1:E:1149:LYS:C    | 2.59                     | 0.45              |
| 1:A:730:ASN:N     | 1:A:730:ASN:HD22  | 2.13                     | 0.45              |
| 1:E:397:ASP:HB2   | 1:E:404:THR:HG22  | 1.99                     | 0.45              |
| 1:E:559:ALA:O     | 1:E:560:MET:HG3   | 2.17                     | 0.45              |
| 1:E:1112:ILE:HG22 | 1:E:1116:LEU:HD13 | 1.97                     | 0.45              |
| 1:A:958:GLY:O     | 3:C:110:DG:H2"    | 2.17                     | 0.45              |
| 1:A:1007:MET:HE1  | 1:A:1055:TYR:CE2  | 2.52                     | 0.45              |
| 1:A:1181:GLN:HB2  | 1:A:1205:THR:CG2  | 2.46                     | 0.45              |
| 1:E:340:VAL:HG21  | 1:E:500:GLU:HG3   | 1.98                     | 0.45              |
| 1:E:985:MET:O     | 1:E:989:GLU:HG3   | 2.17                     | 0.45              |
| 4:A:1301:2ZE:CAS  | 4:A:1301:2ZE:CAW  | 2.91                     | 0.45              |
| 1:E:346:LEU:HB3   | 1:E:689:MET:CE    | 2.40                     | 0.45              |
| 1:E:353:TYR:C     | 1:E:354:ASN:HD22  | 2.25                     | 0.45              |
| 1:E:408:ILE:CD1   | 1:E:472:THR:HA    | 2.46                     | 0.45              |
| 1:E:605:LYS:HB2   | 1:E:607:VAL:HG23  | 1.99                     | 0.45              |
| 1:E:784:ARG:HG2   | 1:E:784:ARG:HH11  | 1.82                     | 0.45              |
| 1:E:788:ASN:ND2   | 1:E:959:CYS:CB    | 2.79                     | 0.45              |
| 1:E:859:LEU:CD2   | 1:E:1040:ILE:HD13 | 2.46                     | 0.45              |
| 1:A:896:GLU:O     | 1:A:897:GLN:HB2   | 2.16                     | 0.45              |
| 1:E:583:PHE:CD2   | 1:E:625:LYS:HE2   | 2.51                     | 0.45              |
| 1:E:601:VAL:O     | 1:E:605:LYS:HG2   | 2.17                     | 0.45              |
| 1:E:1170:LYS:O    | 1:E:1171:ALA:C    | 2.59                     | 0.45              |
| 1:A:1000:TYR:CG   | 1:A:1001:GLY:N    | 2.85                     | 0.44              |
| 1:E:861:PHE:HA    | 1:E:1038:ILE:HA   | 1.98                     | 0.44              |
| 1:A:519:MET:HE1   | 1:A:521:LEU:HD21  | 1.99                     | 0.44              |
| 1:A:1048:LEU:HG   | 1:A:1050:LEU:CD2  | 2.47                     | 0.44              |
| 1:E:409:SER:O     | 1:E:410:MET:C     | 2.57                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:358:VAL:HG22  | 1:A:381:LYS:HG2   | 1.98                     | 0.44              |
| 1:E:727:ASN:O     | 1:E:731:MET:HG3   | 2.17                     | 0.44              |
| 1:E:1128:VAL:HB   | 1:E:1133:PHE:HZ   | 1.81                     | 0.44              |
| 1:A:685:THR:O     | 1:A:686:CYS:C     | 2.60                     | 0.44              |
| 1:A:935:ASN:O     | 1:A:938:LEU:HB2   | 2.17                     | 0.44              |
| 1:E:596:TYR:O     | 1:E:597:ALA:HB3   | 2.18                     | 0.44              |
| 1:E:731:MET:HE2   | 1:E:741:LEU:HB2   | 1.99                     | 0.44              |
| 1:E:1231:ASP:OD2  | 1:E:1233:VAL:HB   | 2.17                     | 0.44              |
| 1:A:1185:ASN:C    | 1:A:1185:ASN:ND2  | 2.66                     | 0.44              |
| 1:E:368:GLU:OE2   | 1:E:368:GLU:HA    | 2.16                     | 0.44              |
| 1:A:718:THR:HG22  | 1:A:719:GLU:N     | 2.32                     | 0.44              |
| 1:E:1142:ASP:O    | 1:E:1144:GLN:N    | 2.51                     | 0.44              |
| 1:A:788:ASN:OD1   | 1:A:956:MET:HE2   | 2.17                     | 0.44              |
| 1:A:806:LYS:HE2   | 1:A:806:LYS:HB3   | 1.80                     | 0.44              |
| 1:A:1139:LEU:N    | 1:A:1139:LEU:HD12 | 2.32                     | 0.44              |
| 1:E:705:SER:HB2   | 1:E:707:HIS:CD2   | 2.52                     | 0.44              |
| 1:E:852:TYR:CE1   | 1:E:999:ILE:HG21  | 2.52                     | 0.44              |
| 1:E:901:LEU:CD2   | 1:E:975:LEU:HD11  | 2.48                     | 0.44              |
| 1:E:978:TYR:C     | 1:E:980:GLY:N     | 2.75                     | 0.44              |
| 1:A:925:VAL:HG13  | 1:A:942:TYR:HB3   | 2.00                     | 0.44              |
| 1:A:1014:ASN:C    | 1:A:1014:ASN:ND2  | 2.76                     | 0.44              |
| 1:E:636:GLY:HA2   | 1:E:752:ILE:HG21  | 2.00                     | 0.44              |
| 1:E:925:VAL:HG21  | 1:E:945:ARG:HG2   | 2.00                     | 0.44              |
| 1:E:937:ASP:HB3   | 5:E:1462:HOH:O    | 2.18                     | 0.44              |
| 1:E:963:SER:HA    | 1:E:968:TYR:CZ    | 2.53                     | 0.44              |
| 1:E:1056:ALA:HB2  | 1:E:1077:LEU:HD11 | 2.00                     | 0.44              |
| 1:A:360:PHE:CE2   | 1:A:379:MET:HE3   | 2.52                     | 0.43              |
| 1:A:1069:VAL:HG12 | 1:A:1070:THR:N    | 2.31                     | 0.43              |
| 1:A:1139:LEU:HD23 | 1:A:1143:PRO:HD3  | 1.99                     | 0.43              |
| 1:A:1148:ASP:O    | 1:A:1149:LYS:C    | 2.62                     | 0.43              |
| 1:E:425:TYR:O     | 1:E:426:LYS:HB2   | 2.18                     | 0.43              |
| 1:E:692:ASP:OD1   | 1:E:692:ASP:C     | 2.60                     | 0.43              |
| 1:E:859:LEU:HD22  | 1:E:1040:ILE:HD13 | 2.00                     | 0.43              |
| 1:E:935:ASN:C     | 1:E:935:ASN:ND2   | 2.75                     | 0.43              |
| 1:E:1149:LYS:HG2  | 1:E:1150:LYS:N    | 2.32                     | 0.43              |
| 1:E:1210:TYR:CD1  | 1:E:1214:GLN:HG3  | 2.53                     | 0.43              |
| 1:E:875:CYS:HB2   | 1:E:912:PRO:CD    | 2.44                     | 0.43              |
| 1:A:1149:LYS:HE3  | 1:A:1159:LEU:HD12 | 1.99                     | 0.43              |
| 1:E:1184:SER:O    | 1:E:1185:ASN:ND2  | 2.52                     | 0.43              |
| 1:A:688:ARG:HH11  | 1:A:688:ARG:HG2   | 1.83                     | 0.43              |
| 1:A:916:ARG:O     | 1:A:920:GLU:HG2   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1010:THR:CG2 | 1:A:1021:LEU:HD23 | 2.44                     | 0.43              |
| 1:A:1182:ASP:OD1 | 1:A:1191:ARG:HG2  | 2.18                     | 0.43              |
| 2:B:3:C:H2'      | 2:B:4:U:C6        | 2.54                     | 0.43              |
| 1:E:645:GLU:O    | 1:E:649:GLN:HG3   | 2.18                     | 0.43              |
| 1:E:672:LYS:NZ   | 1:E:672:LYS:CB    | 2.81                     | 0.43              |
| 1:E:679:PHE:CD2  | 1:E:680:GLY:N     | 2.86                     | 0.43              |
| 1:E:1215:GLN:O   | 1:E:1218:PRO:HD2  | 2.19                     | 0.43              |
| 1:A:762:LEU:HB2  | 1:A:763:PRO:HD3   | 2.01                     | 0.43              |
| 1:A:903:ASP:C    | 1:A:905:SER:H     | 2.26                     | 0.43              |
| 1:E:412:ASP:HB3  | 1:E:472:THR:HG21  | 2.01                     | 0.43              |
| 1:E:578:PRO:HB2  | 1:E:753:LEU:HD21  | 2.01                     | 0.43              |
| 1:E:925:VAL:CG1  | 1:E:942:TYR:HB3   | 2.49                     | 0.43              |
| 1:E:992:GLN:O    | 1:E:995:ASN:N     | 2.51                     | 0.43              |
| 1:E:1018:VAL:O   | 1:E:1021:LEU:HB3  | 2.19                     | 0.43              |
| 1:A:395:LYS:CB   | 1:A:408:ILE:HD11  | 2.48                     | 0.43              |
| 1:A:429:LYS:HD2  | 1:A:429:LYS:N     | 2.33                     | 0.43              |
| 1:A:531:ASP:OD1  | 1:A:531:ASP:N     | 2.45                     | 0.43              |
| 1:A:1014:ASN:C   | 1:A:1014:ASN:HD22 | 2.26                     | 0.43              |
| 1:E:908:MET:CE   | 1:E:916:ARG:HD3   | 2.44                     | 0.43              |
| 1:A:570:LEU:CD2  | 1:A:762:LEU:HB3   | 2.46                     | 0.43              |
| 1:A:625:LYS:O    | 1:A:629:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:901:LEU:HD23 | 1:A:975:LEU:HD21  | 2.01                     | 0.43              |
| 1:A:1053:LYS:O   | 1:A:1054:LYS:HG3  | 2.19                     | 0.43              |
| 1:A:1103:GLN:HB3 | 1:A:1107:THR:HB   | 1.99                     | 0.43              |
| 3:G:316:DC:H2''  | 3:G:317:DC:H5'    | 1.99                     | 0.43              |
| 1:A:1107:THR:O   | 1:A:1111:ASN:ND2  | 2.51                     | 0.43              |
| 4:A:1301:2ZE:H28 | 4:A:1301:2ZE:H16  | 1.80                     | 0.43              |
| 1:E:392:ARG:HB2  | 1:E:408:ILE:HD12  | 2.00                     | 0.43              |
| 1:E:807:GLN:C    | 1:E:808:ILE:HG13  | 2.44                     | 0.43              |
| 1:E:1139:LEU:N   | 1:E:1139:LEU:HD12 | 2.34                     | 0.43              |
| 1:A:935:ASN:HD22 | 1:A:935:ASN:C     | 2.25                     | 0.43              |
| 1:A:1196:GLU:CG  | 1:A:1197:GLN:N    | 2.81                     | 0.43              |
| 1:A:1234:LEU:CG  | 1:A:1238:TRP:CZ2  | 2.99                     | 0.43              |
| 1:E:537:LEU:HD11 | 1:E:570:LEU:HD11  | 2.00                     | 0.43              |
| 1:E:1026:LYS:HG2 | 1:E:1027:SER:N    | 2.34                     | 0.43              |
| 1:A:915:ILE:O    | 1:A:919:VAL:HG23  | 2.19                     | 0.43              |
| 2:B:1:G:H2'      | 2:B:2:C:C6        | 2.53                     | 0.43              |
| 1:E:544:MET:HE1  | 1:E:647:LEU:HB2   | 2.00                     | 0.43              |
| 1:A:444:PRO:O    | 1:A:445:ASP:HB2   | 2.18                     | 0.42              |
| 1:A:1121:GLU:O   | 1:A:1125:ASN:ND2  | 2.52                     | 0.42              |
| 1:E:1046:SER:OG  | 1:E:1058:LEU:HD12 | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:857:LEU:HD11  | 1:E:1022:GLY:N    | 2.34                     | 0.42              |
| 1:E:898:ILE:HA    | 1:E:899:PRO:HD2   | 1.90                     | 0.42              |
| 1:E:1201:GLN:HG2  | 1:E:1203:ASN:OD1  | 2.19                     | 0.42              |
| 1:E:1210:TYR:CD2  | 1:E:1210:TYR:C    | 2.97                     | 0.42              |
| 1:A:1148:ASP:OD1  | 1:A:1148:ASP:O    | 2.36                     | 0.42              |
| 1:E:699:GLU:HG3   | 1:E:784:ARG:HH21  | 1.85                     | 0.42              |
| 1:E:922:ARG:CG    | 1:E:946:GLN:NE2   | 2.71                     | 0.42              |
| 1:E:1222:ARG:NH1  | 3:G:317:DC:OP1    | 2.49                     | 0.42              |
| 3:G:315:DT:C2'    | 3:G:316:DC:C5'    | 2.84                     | 0.42              |
| 1:A:602:ILE:O     | 1:A:603:GLU:C     | 2.63                     | 0.42              |
| 1:A:621:PHE:O     | 1:A:625:LYS:HG2   | 2.19                     | 0.42              |
| 1:A:1139:LEU:HD11 | 1:A:1175:VAL:CG2  | 2.50                     | 0.42              |
| 1:A:1147:PRO:C    | 1:A:1149:LYS:H    | 2.26                     | 0.42              |
| 1:E:503:SER:N     | 1:E:504:PRO:CD    | 2.82                     | 0.42              |
| 1:E:726:GLU:C     | 1:E:728:ILE:N     | 2.77                     | 0.42              |
| 1:E:1185:ASN:C    | 1:E:1185:ASN:ND2  | 2.74                     | 0.42              |
| 1:A:632:ASP:C     | 1:A:633:ILE:HG13  | 2.44                     | 0.42              |
| 1:A:713:GLN:O     | 1:A:717:LYS:HA    | 2.20                     | 0.42              |
| 1:A:1197:GLN:O    | 1:A:1204:LEU:HD12 | 2.20                     | 0.42              |
| 1:A:726:GLU:H     | 1:A:726:GLU:HG3   | 1.62                     | 0.42              |
| 1:A:922:ARG:O     | 1:A:926:LYS:HG3   | 2.20                     | 0.42              |
| 1:E:721:VAL:HG12  | 1:E:722:VAL:N     | 2.34                     | 0.42              |
| 1:E:726:GLU:C     | 1:E:728:ILE:H     | 2.26                     | 0.42              |
| 1:E:392:ARG:HD3   | 1:E:396:ILE:HD13  | 2.02                     | 0.42              |
| 1:E:545:LYS:HG3   | 1:E:741:LEU:HD11  | 2.01                     | 0.42              |
| 1:E:558:ILE:HD12  | 1:E:558:ILE:C     | 2.45                     | 0.42              |
| 1:E:807:GLN:HG2   | 1:E:808:ILE:N     | 2.34                     | 0.42              |
| 1:A:635:VAL:HA    | 1:A:691:CYS:O     | 2.20                     | 0.42              |
| 1:A:1158:ALA:HB2  | 1:A:1175:VAL:HG21 | 2.01                     | 0.42              |
| 1:A:678:GLY:O     | 1:A:682:ARG:HB2   | 2.19                     | 0.42              |
| 1:E:439:TYR:CZ    | 1:E:441:PHE:HB2   | 2.54                     | 0.42              |
| 1:E:593:ILE:O     | 1:E:593:ILE:HG13  | 2.18                     | 0.42              |
| 1:E:784:ARG:HG3   | 3:G:310:DG:C5     | 2.55                     | 0.42              |
| 4:E:1301:2ZE:H30  | 4:E:1301:2ZE:H22  | 1.82                     | 0.42              |
| 1:A:1011:ASN:HD22 | 1:A:1011:ASN:HA   | 1.68                     | 0.41              |
| 1:A:1147:PRO:HG2  | 1:A:1148:ASP:H    | 1.83                     | 0.41              |
| 1:E:522:LYS:O     | 1:E:525:LEU:HB2   | 2.20                     | 0.41              |
| 1:A:593:ILE:O     | 1:A:593:ILE:HG13  | 2.19                     | 0.41              |
| 1:A:605:LYS:HE2   | 1:A:739:LEU:HD23  | 2.01                     | 0.41              |
| 1:A:784:ARG:O     | 1:A:785:SER:C     | 2.63                     | 0.41              |
| 1:A:1209:GLN:HE22 | 1:A:1241:LEU:HD22 | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1152:LEU:HA   | 1:E:1153:PRO:HD2  | 1.79                     | 0.41              |
| 3:G:311:DG:H2'    | 3:G:312:DC:C6     | 2.54                     | 0.41              |
| 1:A:922:ARG:NH2   | 1:A:950:LYS:HD2   | 2.35                     | 0.41              |
| 1:A:1058:LEU:HB3  | 1:A:1070:THR:OG1  | 2.21                     | 0.41              |
| 1:A:1139:LEU:HD11 | 1:A:1175:VAL:HG23 | 2.02                     | 0.41              |
| 4:A:1301:2ZE:H22  | 4:A:1301:2ZE:H30  | 1.72                     | 0.41              |
| 1:E:507:LEU:O     | 1:E:508:ASN:C     | 2.62                     | 0.41              |
| 1:E:730:ASN:HD22  | 1:E:730:ASN:H     | 1.55                     | 0.41              |
| 1:E:788:ASN:HB2   | 1:E:959:CYS:SG    | 2.60                     | 0.41              |
| 1:A:627:HIS:HB2   | 1:A:661:LYS:HD3   | 2.03                     | 0.41              |
| 1:A:1092:GLY:O    | 1:A:1096:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:1170:LYS:O    | 1:A:1171:ALA:C    | 2.63                     | 0.41              |
| 1:E:667:ARG:HH22  | 1:E:683:ASN:HB3   | 1.84                     | 0.41              |
| 1:E:988:LYS:HG3   | 1:E:998:VAL:HG11  | 2.01                     | 0.41              |
| 1:E:1082:ARG:HG3  | 1:E:1136:ASN:HB2  | 2.02                     | 0.41              |
| 1:A:908:MET:HB3   | 1:A:913:ARG:HD3   | 2.03                     | 0.41              |
| 1:A:1054:LYS:HA   | 1:A:1075:LYS:O    | 2.21                     | 0.41              |
| 1:A:1170:LYS:HG2  | 1:A:1173:ASP:OD2  | 2.21                     | 0.41              |
| 1:E:654:CYS:O     | 1:E:655:LYS:C     | 2.63                     | 0.41              |
| 1:E:791:LEU:HD12  | 1:E:791:LEU:O     | 2.20                     | 0.41              |
| 1:E:865:TYR:CB    | 1:E:866:PRO:HD3   | 2.49                     | 0.41              |
| 1:E:873:ASN:HD21  | 1:E:878:THR:HG21  | 1.85                     | 0.41              |
| 1:E:1006:ILE:HA   | 1:E:1006:ILE:HD13 | 1.81                     | 0.41              |
| 1:A:721:VAL:HG12  | 1:A:722:VAL:N     | 2.36                     | 0.41              |
| 1:A:1082:ARG:HG3  | 1:A:1136:ASN:HB2  | 2.02                     | 0.41              |
| 3:C:110:DG:N3     | 3:C:110:DG:H3'    | 2.36                     | 0.41              |
| 1:A:596:TYR:O     | 1:A:597:ALA:HB3   | 2.21                     | 0.41              |
| 4:A:1301:2ZE:H13  | 4:A:1301:2ZE:H21  | 1.87                     | 0.41              |
| 1:E:1103:GLN:HB3  | 1:E:1107:THR:HB   | 2.03                     | 0.41              |
| 1:A:588:LYS:HA    | 1:A:732:TYR:HE2   | 1.85                     | 0.41              |
| 1:A:667:ARG:HH22  | 1:A:683:ASN:HB3   | 1.86                     | 0.41              |
| 1:A:705:SER:HB3   | 1:A:1174:THR:OG1  | 2.20                     | 0.41              |
| 1:A:1138:ALA:HA   | 1:A:1174:THR:HA   | 2.02                     | 0.41              |
| 1:A:1152:LEU:HD13 | 2:B:6:G:H4'       | 2.03                     | 0.41              |
| 2:B:2:C:O2'       | 2:B:3:C:H5'       | 2.21                     | 0.41              |
| 3:C:118:DA:H2''   | 3:C:119:DG:C5'    | 2.43                     | 0.41              |
| 1:E:360:PHE:CZ    | 1:E:379:MET:HE3   | 2.56                     | 0.41              |
| 1:E:593:ILE:O     | 1:E:594:PHE:C     | 2.62                     | 0.41              |
| 1:E:723:ILE:HD13  | 1:E:731:MET:HE1   | 2.03                     | 0.41              |
| 1:E:1053:LYS:HD3  | 2:F:210:G:H1'     | 2.03                     | 0.41              |
| 4:E:1301:2ZE:CAS  | 4:E:1301:2ZE:CAW  | 2.94                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:649:GLN:O     | 1:A:653:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:849:VAL:HG12  | 1:A:850:GLY:N    | 2.36                     | 0.41              |
| 1:A:1169:VAL:HG13 | 1:A:1173:ASP:HB2 | 2.03                     | 0.41              |
| 1:E:586:VAL:CB    | 1:E:742:LEU:HD21 | 2.51                     | 0.41              |
| 1:A:549:ASN:OD1   | 1:A:552:ASN:O    | 2.39                     | 0.40              |
| 1:A:922:ARG:NH2   | 1:A:946:GLN:OE1  | 2.51                     | 0.40              |
| 1:A:1202:ASP:C    | 1:A:1204:LEU:H   | 2.29                     | 0.40              |
| 1:E:433:LYS:HB3   | 1:E:433:LYS:HE2  | 1.92                     | 0.40              |
| 1:E:970:LYS:N     | 1:E:971:PRO:CD   | 2.85                     | 0.40              |
| 1:E:1142:ASP:HB2  | 1:E:1145:ASP:OD2 | 2.21                     | 0.40              |
| 4:E:1301:2ZE:H21  | 4:E:1301:2ZE:H13 | 1.90                     | 0.40              |
| 1:A:1166:GLY:O    | 1:A:1167:ARG:C   | 2.64                     | 0.40              |
| 1:E:678:GLY:HA2   | 1:E:681:GLU:OE1  | 2.22                     | 0.40              |
| 1:E:854:LYS:HB3   | 1:E:1012:SER:O   | 2.21                     | 0.40              |
| 1:E:1050:LEU:HD13 | 1:E:1222:ARG:O   | 2.21                     | 0.40              |
| 1:E:1082:ARG:CG   | 1:E:1136:ASN:HB2 | 2.51                     | 0.40              |
| 1:E:1179:ILE:HD12 | 1:E:1188:ALA:O   | 2.21                     | 0.40              |
| 2:F:210:G:H2'     | 2:F:211:DC:C6    | 2.56                     | 0.40              |
| 1:A:588:LYS:HA    | 1:A:732:TYR:CE2  | 2.56                     | 0.40              |
| 1:E:685:THR:O     | 1:E:686:CYS:C    | 2.65                     | 0.40              |
| 1:E:705:SER:OG    | 1:E:710:GLU:HG2  | 2.21                     | 0.40              |
| 1:E:1237:THR:HG23 | 1:E:1243:PRO:HG3 | 2.02                     | 0.40              |
| 1:E:633:ILE:HD13  | 1:E:762:LEU:HD22 | 2.04                     | 0.40              |
| 1:E:990:MET:HG2   | 1:E:994:MET:HE3  | 2.04                     | 0.40              |
| 1:A:521:LEU:HD23  | 1:A:521:LEU:HA   | 1.94                     | 0.40              |
| 1:A:669:ASN:N     | 1:A:669:ASN:ND2  | 2.69                     | 0.40              |
| 1:A:1139:LEU:CD2  | 1:A:1143:PRO:HD3 | 2.51                     | 0.40              |
| 1:A:1149:LYS:HE3  | 1:A:1159:LEU:CD1 | 2.51                     | 0.40              |
| 1:E:345:TRP:HA    | 1:E:363:GLY:HA3  | 2.04                     | 0.40              |
| 1:E:447:PRO:HB2   | 1:E:449:LYS:O    | 2.21                     | 0.40              |
| 1:E:1116:LEU:HD22 | 1:E:1238:TRP:HE3 | 1.87                     | 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     | 857/922 (93%)   | 785 (92%)  | 56 (6%)  | 16 (2%)  | 6           | 10 |
| 1   | E     | 857/922 (93%)   | 783 (91%)  | 62 (7%)  | 12 (1%)  | 9           | 16 |
| All | All   | 1714/1844 (93%) | 1568 (92%) | 118 (7%) | 28 (2%)  | 7           | 13 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 551  | LYS  |
| 1   | A     | 553  | HIS  |
| 1   | A     | 589  | PRO  |
| 1   | A     | 1101 | SER  |
| 1   | A     | 1149 | LYS  |
| 1   | E     | 551  | LYS  |
| 1   | E     | 1101 | SER  |
| 1   | E     | 1149 | LYS  |
| 1   | A     | 849  | VAL  |
| 1   | A     | 897  | GLN  |
| 1   | A     | 1003 | THR  |
| 1   | A     | 1150 | LYS  |
| 1   | E     | 589  | PRO  |
| 1   | E     | 1150 | LYS  |
| 1   | E     | 1003 | THR  |
| 1   | A     | 1103 | GLN  |
| 1   | E     | 1143 | PRO  |
| 1   | E     | 1166 | GLY  |
| 1   | A     | 1243 | PRO  |
| 1   | E     | 462  | PRO  |
| 1   | A     | 1153 | PRO  |
| 1   | E     | 399  | ASN  |
| 1   | E     | 1026 | LYS  |
| 1   | A     | 1166 | GLY  |
| 1   | A     | 462  | PRO  |
| 1   | A     | 1143 | PRO  |
| 1   | A     | 1147 | PRO  |
| 1   | E     | 1243 | 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     | 778/827 (94%)   | 736 (95%)  | 42 (5%)  | 20          | 39 |
| 1   | E     | 778/827 (94%)   | 730 (94%)  | 48 (6%)  | 16          | 32 |
| All | All   | 1556/1654 (94%) | 1466 (94%) | 90 (6%)  | 18          | 36 |

All (90) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 343 | PHE  |
| 1   | A     | 350 | GLU  |
| 1   | A     | 354 | ASN  |
| 1   | A     | 355 | GLN  |
| 1   | A     | 365 | VAL  |
| 1   | A     | 406 | THR  |
| 1   | A     | 451 | GLU  |
| 1   | A     | 458 | SER  |
| 1   | A     | 484 | LEU  |
| 1   | A     | 529 | ILE  |
| 1   | A     | 555 | ASN  |
| 1   | A     | 567 | SER  |
| 1   | A     | 606 | ASN  |
| 1   | A     | 609 | VAL  |
| 1   | A     | 611 | VAL  |
| 1   | A     | 635 | VAL  |
| 1   | A     | 668 | SER  |
| 1   | A     | 726 | GLU  |
| 1   | A     | 727 | ASN  |
| 1   | A     | 729 | GLN  |
| 1   | A     | 739 | LEU  |
| 1   | A     | 764 | LEU  |
| 1   | A     | 785 | SER  |
| 1   | A     | 852 | TYR  |
| 1   | A     | 860 | ASP  |
| 1   | A     | 898 | ILE  |
| 1   | A     | 908 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 912  | PRO  |
| 1   | A     | 933  | ASP  |
| 1   | A     | 935  | ASN  |
| 1   | A     | 937  | ASP  |
| 1   | A     | 938  | LEU  |
| 1   | A     | 956  | MET  |
| 1   | A     | 1039 | ASP  |
| 1   | A     | 1080 | VAL  |
| 1   | A     | 1082 | ARG  |
| 1   | A     | 1098 | GLN  |
| 1   | A     | 1111 | ASN  |
| 1   | A     | 1185 | ASN  |
| 1   | A     | 1199 | GLN  |
| 1   | A     | 1231 | ASP  |
| 1   | A     | 1243 | PRO  |
| 1   | E     | 343  | PHE  |
| 1   | E     | 354  | ASN  |
| 1   | E     | 359  | VAL  |
| 1   | E     | 365  | VAL  |
| 1   | E     | 372  | THR  |
| 1   | E     | 393  | GLU  |
| 1   | E     | 406  | THR  |
| 1   | E     | 529  | ILE  |
| 1   | E     | 546  | THR  |
| 1   | E     | 548  | GLN  |
| 1   | E     | 552  | ASN  |
| 1   | E     | 554  | GLN  |
| 1   | E     | 555  | ASN  |
| 1   | E     | 567  | SER  |
| 1   | E     | 596  | TYR  |
| 1   | E     | 609  | VAL  |
| 1   | E     | 611  | VAL  |
| 1   | E     | 618  | LEU  |
| 1   | E     | 669  | ASN  |
| 1   | E     | 672  | LYS  |
| 1   | E     | 727  | ASN  |
| 1   | E     | 728  | ILE  |
| 1   | E     | 730  | ASN  |
| 1   | E     | 742  | LEU  |
| 1   | E     | 764  | LEU  |
| 1   | E     | 784  | ARG  |
| 1   | E     | 857  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 860  | ASP  |
| 1   | E     | 866  | PRO  |
| 1   | E     | 913  | ARG  |
| 1   | E     | 916  | ARG  |
| 1   | E     | 927  | GLN  |
| 1   | E     | 935  | ASN  |
| 1   | E     | 938  | LEU  |
| 1   | E     | 943  | ASP  |
| 1   | E     | 944  | ILE  |
| 1   | E     | 945  | ARG  |
| 1   | E     | 1006 | ILE  |
| 1   | E     | 1011 | ASN  |
| 1   | E     | 1039 | ASP  |
| 1   | E     | 1047 | LEU  |
| 1   | E     | 1098 | GLN  |
| 1   | E     | 1173 | ASP  |
| 1   | E     | 1185 | ASN  |
| 1   | E     | 1198 | LEU  |
| 1   | E     | 1199 | GLN  |
| 1   | E     | 1231 | ASP  |
| 1   | E     | 1242 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 354 | ASN  |
| 1   | A     | 355 | GLN  |
| 1   | A     | 548 | GLN  |
| 1   | A     | 554 | GLN  |
| 1   | A     | 555 | ASN  |
| 1   | A     | 606 | ASN  |
| 1   | A     | 649 | GLN  |
| 1   | A     | 652 | ASN  |
| 1   | A     | 669 | ASN  |
| 1   | A     | 683 | ASN  |
| 1   | A     | 727 | ASN  |
| 1   | A     | 729 | GLN  |
| 1   | A     | 730 | ASN  |
| 1   | A     | 754 | GLN  |
| 1   | A     | 760 | ASN  |
| 1   | A     | 770 | ASN  |
| 1   | A     | 870 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 880  | GLN  |
| 1   | A     | 897  | GLN  |
| 1   | A     | 927  | GLN  |
| 1   | A     | 931  | GLN  |
| 1   | A     | 932  | GLN  |
| 1   | A     | 935  | ASN  |
| 1   | A     | 954  | ASN  |
| 1   | A     | 986  | HIS  |
| 1   | A     | 1011 | ASN  |
| 1   | A     | 1098 | GLN  |
| 1   | A     | 1103 | GLN  |
| 1   | A     | 1111 | ASN  |
| 1   | A     | 1113 | GLN  |
| 1   | A     | 1125 | ASN  |
| 1   | A     | 1132 | GLN  |
| 1   | A     | 1144 | GLN  |
| 1   | A     | 1181 | GLN  |
| 1   | A     | 1185 | ASN  |
| 1   | A     | 1199 | GLN  |
| 1   | A     | 1201 | GLN  |
| 1   | A     | 1209 | GLN  |
| 1   | E     | 354  | ASN  |
| 1   | E     | 475  | HIS  |
| 1   | E     | 548  | GLN  |
| 1   | E     | 554  | GLN  |
| 1   | E     | 555  | ASN  |
| 1   | E     | 606  | ASN  |
| 1   | E     | 649  | GLN  |
| 1   | E     | 652  | ASN  |
| 1   | E     | 658  | HIS  |
| 1   | E     | 669  | ASN  |
| 1   | E     | 683  | ASN  |
| 1   | E     | 707  | HIS  |
| 1   | E     | 713  | GLN  |
| 1   | E     | 727  | ASN  |
| 1   | E     | 730  | ASN  |
| 1   | E     | 754  | GLN  |
| 1   | E     | 770  | ASN  |
| 1   | E     | 788  | ASN  |
| 1   | E     | 800  | ASN  |
| 1   | E     | 870  | GLN  |
| 1   | E     | 880  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 897  | GLN  |
| 1   | E     | 924  | GLN  |
| 1   | E     | 931  | GLN  |
| 1   | E     | 932  | GLN  |
| 1   | E     | 935  | ASN  |
| 1   | E     | 941  | GLN  |
| 1   | E     | 946  | GLN  |
| 1   | E     | 954  | ASN  |
| 1   | E     | 1011 | ASN  |
| 1   | E     | 1014 | ASN  |
| 1   | E     | 1072 | GLN  |
| 1   | E     | 1093 | ASN  |
| 1   | E     | 1111 | ASN  |
| 1   | E     | 1113 | GLN  |
| 1   | E     | 1122 | ASN  |
| 1   | E     | 1132 | GLN  |
| 1   | E     | 1156 | HIS  |
| 1   | E     | 1181 | GLN  |
| 1   | E     | 1185 | ASN  |
| 1   | E     | 1199 | GLN  |
| 1   | E     | 1201 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | B     | 9/11 (81%)  | 0                 | 0               |
| 2   | F     | 9/11 (81%)  | 0                 | 0               |
| All | All   | 18/22 (81%) | 0                 | 0               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | 2ZE  | E     | 1301 | -    | 27,27,27     | 1.08 | 4 (14%)  | 44,46,46    | 1.63 | 5 (11%)  |
| 4   | 2ZE  | A     | 1301 | -    | 27,27,27     | 1.08 | 4 (14%)  | 44,46,46    | 1.61 | 7 (15%)  |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 4   | 2ZE  | E     | 1301 | -    | -       | 3/6/72/72 | 0/5/4/4 |
| 4   | 2ZE  | A     | 1301 | -    | -       | 3/6/72/72 | 0/5/4/4 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | E     | 1301 | 2ZE  | CAF-CAE | -2.79 | 1.52        | 1.57     |
| 4   | A     | 1301 | 2ZE  | CAF-CAE | -2.73 | 1.52        | 1.57     |
| 4   | A     | 1301 | 2ZE  | CAF-CAH | -2.45 | 1.52        | 1.56     |
| 4   | E     | 1301 | 2ZE  | CAE-CAG | -2.41 | 1.51        | 1.55     |
| 4   | E     | 1301 | 2ZE  | CAN-CAH | -2.32 | 1.53        | 1.56     |
| 4   | A     | 1301 | 2ZE  | CAN-CAH | -2.28 | 1.53        | 1.56     |
| 4   | A     | 1301 | 2ZE  | CAE-CAG | -2.21 | 1.52        | 1.55     |
| 4   | E     | 1301 | 2ZE  | CAF-CAH | -2.01 | 1.53        | 1.56     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | A     | 1301 | 2ZE  | CAL-CAE-CAI | 5.85  | 111.50      | 105.19   |
| 4   | E     | 1301 | 2ZE  | CAL-CAE-CAI | 5.80  | 111.46      | 105.19   |
| 4   | A     | 1301 | 2ZE  | CAK-CAJ-CAP | -3.41 | 107.84      | 111.07   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | E     | 1301 | 2ZE  | CAK-CAJ-CAP | -3.36 | 107.89      | 111.07   |
| 4   | E     | 1301 | 2ZE  | CAF-CAH-CAN | -2.95 | 113.37      | 116.75   |
| 4   | A     | 1301 | 2ZE  | CAF-CAH-CAN | -2.95 | 113.37      | 116.75   |
| 4   | A     | 1301 | 2ZE  | CAU-CAT-CAN | -2.90 | 110.00      | 113.13   |
| 4   | E     | 1301 | 2ZE  | CAU-CAT-CAN | -2.64 | 110.28      | 113.13   |
| 4   | E     | 1301 | 2ZE  | CAI-CAJ-CAP | -2.29 | 108.31      | 110.17   |
| 4   | A     | 1301 | 2ZE  | CAI-CAE-CAG | -2.09 | 97.28       | 100.14   |
| 4   | A     | 1301 | 2ZE  | CAO-CAH-CAN | -2.08 | 111.53      | 114.31   |
| 4   | A     | 1301 | 2ZE  | CAU-CAQ-CAF | -2.03 | 109.35      | 112.85   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

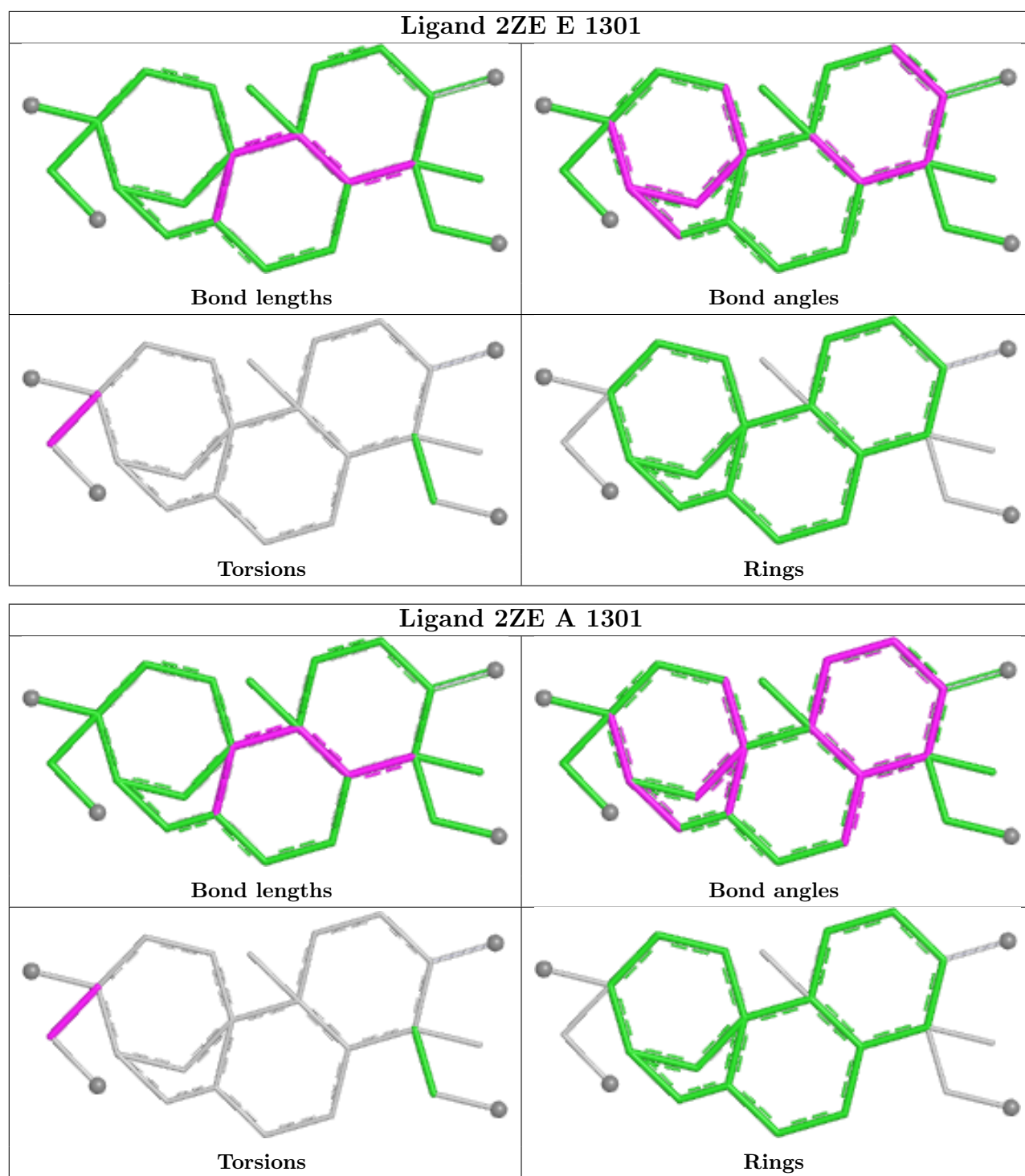
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | A     | 1301 | 2ZE  | CAJ-CAP-CAX-OAD |
| 4   | E     | 1301 | 2ZE  | CAJ-CAP-CAX-OAD |
| 4   | E     | 1301 | 2ZE  | CAR-CAP-CAX-OAD |
| 4   | E     | 1301 | 2ZE  | OAA-CAP-CAX-OAD |
| 4   | A     | 1301 | 2ZE  | CAR-CAP-CAX-OAD |
| 4   | A     | 1301 | 2ZE  | OAA-CAP-CAX-OAD |

There are no ring outliers.

2 monomers are involved in 14 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | E     | 1301 | 2ZE  | 6       | 0            |
| 4   | A     | 1301 | 2ZE  | 8       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 865/922 (93%)   | 0.59   | 109 (12%) 8 6  | 15, 54, 113, 128      | 0     |
| 1   | E     | 865/922 (93%)   | 0.55   | 92 (10%) 11 9  | 18, 52, 105, 129      | 0     |
| 2   | B     | 11/11 (100%)    | 0.01   | 0 100 100      | 48, 62, 78, 87        | 0     |
| 2   | F     | 11/11 (100%)    | -0.15  | 0 100 100      | 43, 52, 79, 81        | 0     |
| 3   | C     | 13/21 (61%)     | 0.13   | 1 (7%) 19 17   | 37, 59, 92, 101       | 0     |
| 3   | G     | 13/21 (61%)     | 0.19   | 1 (7%) 19 17   | 42, 57, 76, 85        | 0     |
| All | All   | 1778/1908 (93%) | 0.56   | 203 (11%) 10 8 | 15, 53, 111, 129      | 0     |

All (203) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 679  | PHE  | 5.8  |
| 1   | A     | 679  | PHE  | 5.8  |
| 1   | A     | 1241 | LEU  | 5.7  |
| 1   | E     | 673  | LEU  | 5.7  |
| 1   | A     | 1239 | LEU  | 5.6  |
| 1   | A     | 673  | LEU  | 5.6  |
| 1   | E     | 808  | ILE  | 5.5  |
| 1   | E     | 882  | VAL  | 5.4  |
| 1   | A     | 1243 | PRO  | 5.1  |
| 1   | A     | 1233 | VAL  | 5.0  |
| 1   | E     | 398  | LEU  | 5.0  |
| 1   | A     | 678  | GLY  | 4.7  |
| 1   | E     | 681  | GLU  | 4.5  |
| 1   | E     | 678  | GLY  | 4.5  |
| 1   | A     | 1230 | ILE  | 4.5  |
| 1   | A     | 671  | PRO  | 4.4  |
| 1   | A     | 1124 | LEU  | 4.4  |
| 1   | E     | 671  | PRO  | 4.3  |
| 1   | E     | 1244 | THR  | 4.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1244 | THR  | 4.1  |
| 1   | A     | 808  | ILE  | 4.1  |
| 1   | A     | 850  | GLY  | 4.1  |
| 1   | E     | 682  | ARG  | 4.1  |
| 1   | E     | 1167 | ARG  | 4.0  |
| 1   | A     | 1180 | CYS  | 3.8  |
| 1   | A     | 672  | LYS  | 3.8  |
| 1   | A     | 1066 | GLY  | 3.7  |
| 1   | E     | 1066 | GLY  | 3.6  |
| 1   | E     | 1124 | LEU  | 3.6  |
| 1   | E     | 1233 | VAL  | 3.6  |
| 1   | E     | 1150 | LYS  | 3.6  |
| 1   | A     | 1117 | ILE  | 3.6  |
| 1   | A     | 882  | VAL  | 3.6  |
| 1   | E     | 933  | ASP  | 3.6  |
| 1   | E     | 1123 | VAL  | 3.5  |
| 1   | A     | 1167 | ARG  | 3.5  |
| 1   | E     | 596  | TYR  | 3.5  |
| 1   | A     | 681  | GLU  | 3.4  |
| 1   | E     | 680  | GLY  | 3.4  |
| 1   | A     | 1212 | LEU  | 3.4  |
| 1   | A     | 1130 | VAL  | 3.3  |
| 1   | E     | 1239 | LEU  | 3.3  |
| 1   | A     | 682  | ARG  | 3.3  |
| 3   | G     | 309  | DA   | 3.3  |
| 1   | A     | 1226 | PRO  | 3.3  |
| 1   | A     | 607  | VAL  | 3.3  |
| 1   | A     | 1070 | THR  | 3.3  |
| 1   | E     | 550  | ALA  | 3.3  |
| 1   | E     | 725  | MET  | 3.3  |
| 1   | A     | 1229 | GLY  | 3.2  |
| 1   | A     | 1126 | GLY  | 3.2  |
| 1   | A     | 1147 | PRO  | 3.1  |
| 1   | A     | 552  | ASN  | 3.1  |
| 1   | A     | 1232 | ALA  | 3.1  |
| 1   | E     | 1213 | ALA  | 3.1  |
| 1   | A     | 1123 | VAL  | 3.1  |
| 1   | E     | 1180 | CYS  | 3.1  |
| 1   | E     | 1243 | PRO  | 3.1  |
| 1   | A     | 1186 | LEU  | 3.1  |
| 1   | E     | 399  | ASN  | 3.1  |
| 1   | E     | 1128 | VAL  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1217 | HIS  | 3.0  |
| 1   | A     | 1217 | HIS  | 3.0  |
| 1   | E     | 896  | GLU  | 3.0  |
| 1   | A     | 590  | LYS  | 3.0  |
| 1   | E     | 404  | THR  | 3.0  |
| 1   | A     | 1183 | GLY  | 3.0  |
| 1   | E     | 1230 | ILE  | 2.9  |
| 1   | A     | 1151 | SER  | 2.9  |
| 1   | A     | 550  | ALA  | 2.9  |
| 1   | E     | 857  | LEU  | 2.9  |
| 1   | A     | 1119 | ILE  | 2.8  |
| 1   | E     | 552  | ASN  | 2.8  |
| 3   | C     | 109  | DA   | 2.8  |
| 1   | A     | 1150 | LYS  | 2.8  |
| 1   | E     | 1232 | ALA  | 2.8  |
| 1   | A     | 1198 | LEU  | 2.8  |
| 1   | E     | 930  | LYS  | 2.8  |
| 1   | A     | 1228 | ASP  | 2.8  |
| 1   | A     | 608  | LYS  | 2.8  |
| 1   | A     | 1235 | ILE  | 2.7  |
| 1   | A     | 1238 | TRP  | 2.7  |
| 1   | A     | 1069 | VAL  | 2.7  |
| 1   | E     | 1237 | THR  | 2.7  |
| 1   | E     | 396  | ILE  | 2.7  |
| 1   | A     | 596  | TYR  | 2.7  |
| 1   | A     | 1193 | TYR  | 2.7  |
| 1   | A     | 1160 | TRP  | 2.7  |
| 1   | A     | 1116 | LEU  | 2.6  |
| 1   | E     | 1117 | ILE  | 2.6  |
| 1   | E     | 726  | GLU  | 2.6  |
| 1   | E     | 1063 | THR  | 2.6  |
| 1   | E     | 1070 | THR  | 2.6  |
| 1   | A     | 1019 | PHE  | 2.6  |
| 1   | E     | 592  | CYS  | 2.6  |
| 1   | A     | 551  | LYS  | 2.6  |
| 1   | E     | 1165 | GLY  | 2.5  |
| 1   | E     | 1183 | GLY  | 2.5  |
| 1   | A     | 730  | ASN  | 2.5  |
| 1   | A     | 1169 | VAL  | 2.5  |
| 1   | E     | 1214 | GLN  | 2.5  |
| 1   | A     | 1205 | THR  | 2.5  |
| 1   | E     | 353  | TYR  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1216 | ILE  | 2.5  |
| 1   | A     | 1234 | LEU  | 2.5  |
| 1   | E     | 1198 | LEU  | 2.5  |
| 1   | E     | 1130 | VAL  | 2.5  |
| 1   | E     | 1143 | PRO  | 2.5  |
| 1   | A     | 680  | GLY  | 2.5  |
| 1   | E     | 1206 | ILE  | 2.5  |
| 1   | E     | 608  | LYS  | 2.5  |
| 1   | A     | 1185 | ASN  | 2.5  |
| 1   | E     | 400  | THR  | 2.5  |
| 1   | E     | 1147 | PRO  | 2.4  |
| 1   | A     | 852  | TYR  | 2.4  |
| 1   | A     | 1149 | LYS  | 2.4  |
| 1   | E     | 402  | LYS  | 2.4  |
| 1   | E     | 1238 | TRP  | 2.4  |
| 1   | A     | 849  | VAL  | 2.4  |
| 1   | E     | 683  | ASN  | 2.4  |
| 1   | E     | 836  | LYS  | 2.4  |
| 1   | E     | 1229 | GLY  | 2.4  |
| 1   | E     | 1227 | ILE  | 2.4  |
| 1   | E     | 1235 | ILE  | 2.4  |
| 1   | A     | 597  | ALA  | 2.4  |
| 1   | E     | 1062 | PRO  | 2.4  |
| 1   | E     | 728  | ILE  | 2.4  |
| 1   | A     | 1105 | ARG  | 2.4  |
| 1   | A     | 1236 | ALA  | 2.4  |
| 1   | E     | 551  | LYS  | 2.4  |
| 1   | E     | 672  | LYS  | 2.4  |
| 1   | E     | 1129 | PRO  | 2.4  |
| 1   | E     | 1144 | GLN  | 2.4  |
| 1   | E     | 553  | HIS  | 2.4  |
| 1   | A     | 1133 | PHE  | 2.4  |
| 1   | A     | 1177 | TYR  | 2.4  |
| 1   | A     | 1211 | TYR  | 2.4  |
| 1   | E     | 401  | GLY  | 2.3  |
| 1   | E     | 1146 | TYR  | 2.3  |
| 1   | A     | 1168 | LYS  | 2.3  |
| 1   | A     | 1046 | SER  | 2.3  |
| 1   | A     | 1144 | GLN  | 2.3  |
| 1   | A     | 1225 | GLU  | 2.3  |
| 1   | E     | 1195 | PRO  | 2.3  |
| 1   | E     | 1215 | GLN  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1048 | LEU  | 2.3  |
| 1   | A     | 1108 | ILE  | 2.3  |
| 1   | A     | 1204 | LEU  | 2.3  |
| 1   | A     | 1206 | ILE  | 2.3  |
| 1   | E     | 934  | LEU  | 2.3  |
| 1   | E     | 1069 | VAL  | 2.3  |
| 1   | E     | 1109 | VAL  | 2.3  |
| 1   | A     | 353  | TYR  | 2.3  |
| 1   | A     | 1210 | TYR  | 2.3  |
| 1   | A     | 1227 | ILE  | 2.2  |
| 1   | A     | 1231 | ASP  | 2.2  |
| 1   | A     | 601  | VAL  | 2.2  |
| 1   | A     | 834  | ARG  | 2.2  |
| 1   | A     | 1062 | PRO  | 2.2  |
| 1   | A     | 1109 | VAL  | 2.2  |
| 1   | E     | 1105 | ARG  | 2.2  |
| 1   | E     | 640  | TYR  | 2.2  |
| 1   | A     | 807  | GLN  | 2.2  |
| 1   | E     | 445  | ASP  | 2.2  |
| 1   | A     | 1094 | PHE  | 2.2  |
| 1   | A     | 705  | SER  | 2.2  |
| 1   | E     | 338  | GLU  | 2.2  |
| 1   | A     | 1100 | LEU  | 2.2  |
| 1   | A     | 1240 | GLY  | 2.2  |
| 1   | A     | 1040 | ILE  | 2.2  |
| 1   | A     | 1220 | VAL  | 2.1  |
| 1   | E     | 722  | VAL  | 2.1  |
| 1   | A     | 554  | GLN  | 2.1  |
| 1   | E     | 932  | GLN  | 2.1  |
| 1   | A     | 1063 | THR  | 2.1  |
| 1   | E     | 1079 | ILE  | 2.1  |
| 1   | A     | 933  | ASP  | 2.1  |
| 1   | E     | 1113 | GLN  | 2.1  |
| 1   | A     | 1192 | ALA  | 2.1  |
| 1   | A     | 592  | CYS  | 2.1  |
| 1   | A     | 1195 | PRO  | 2.1  |
| 1   | A     | 1060 | VAL  | 2.1  |
| 1   | A     | 1128 | VAL  | 2.1  |
| 1   | E     | 1169 | VAL  | 2.1  |
| 1   | E     | 1186 | LEU  | 2.1  |
| 1   | E     | 782  | GLY  | 2.1  |
| 1   | E     | 1161 | ILE  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1071 | LYS  | 2.1  |
| 1   | E     | 1148 | ASP  | 2.1  |
| 1   | A     | 1224 | CYS  | 2.1  |
| 1   | E     | 589  | PRO  | 2.1  |
| 1   | E     | 607  | VAL  | 2.0  |
| 1   | E     | 730  | ASN  | 2.0  |
| 1   | E     | 1204 | LEU  | 2.0  |
| 1   | A     | 605  | LYS  | 2.0  |
| 1   | A     | 836  | LYS  | 2.0  |
| 1   | E     | 1210 | TYR  | 2.0  |
| 1   | A     | 722  | VAL  | 2.0  |
| 1   | A     | 1087 | LEU  | 2.0  |
| 1   | A     | 728  | ILE  | 2.0  |
| 1   | A     | 1187 | THR  | 2.0  |
| 1   | A     | 1223 | ILE  | 2.0  |
| 1   | A     | 990  | MET  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

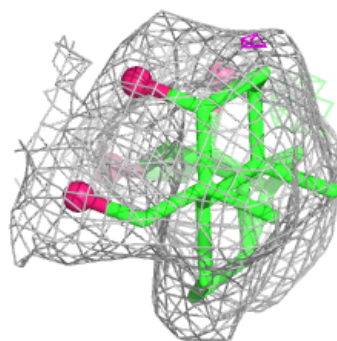
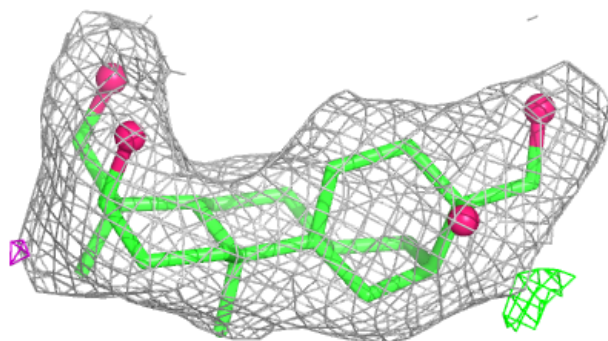
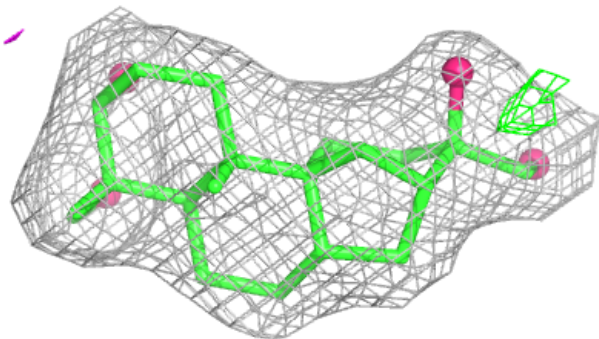
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | 2ZE  | A     | 1301 | 24/24 | 0.94 | 0.09 | 20,29,34,42                 | 0     |
| 4   | 2ZE  | E     | 1301 | 24/24 | 0.95 | 0.08 | 30,37,43,43                 | 0     |

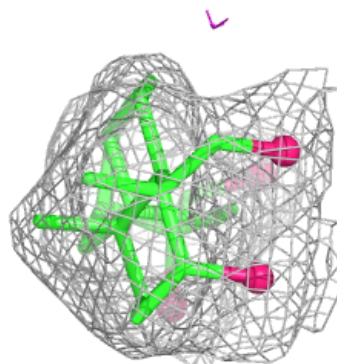
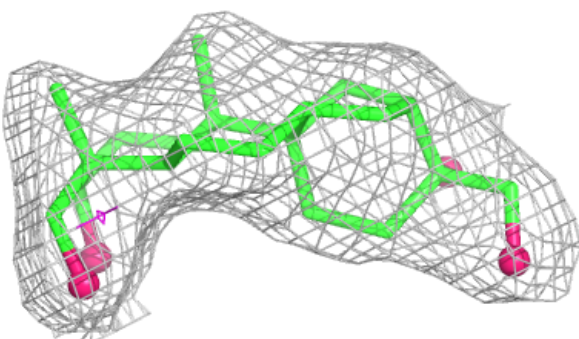
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2ZE A 1301:**

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

**Electron density around 2ZE E 1301:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.