



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GMO  
Title : CRYSTAL STRUCTURES OF NK1-HEPARIN COMPLEXES REVEAL THE BASIS FOR NK1 ACTIVITY AND ENABLE ENGINEERING OF POTENT AGONISTS OF THE MET RECEPTOR  
Authors : Lietha, D.; Chirgadze, D.Y.; Mulloy, B.; Blundell, T.L.; Gherardi, E.  
Deposited on : 2001-09-20  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

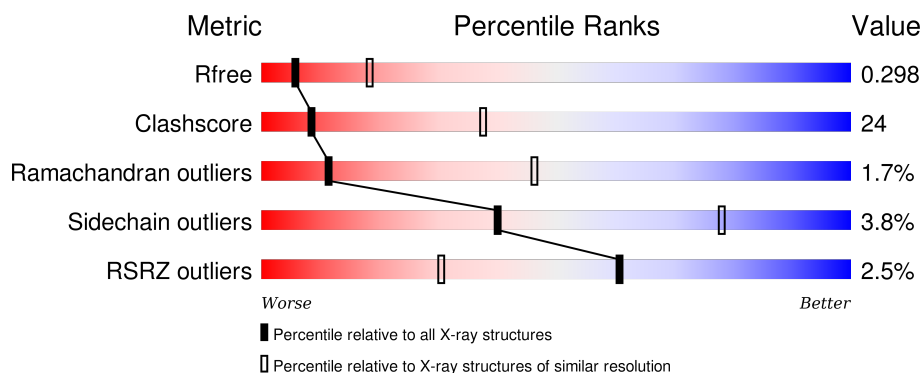
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1578 (3.00-3.00)                                      |
| Clashscore            | 102246                      | 1912 (3.00-3.00)                                      |
| Ramachandran outliers | 100387                      | 1853 (3.00-3.00)                                      |
| Sidechain outliers    | 100360                      | 1856 (3.00-3.00)                                      |
| RSRZ outliers         | 91569                       | 1592 (3.00-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 183    | <div> <div>4%</div> <div>56%</div> <div>34%</div> <div>6%</div> </div> |
| 1   | B     | 183    | <div> <div>%</div> <div>58%</div> <div>34%</div> <div>6%</div> </div>  |
| 1   | C     | 183    | <div> <div>54%</div> <div>38%</div> <div>6%</div> </div>               |
| 1   | D     | 183    | <div> <div>%</div> <div>52%</div> <div>38%</div> <div>6%</div> </div>  |
| 1   | E     | 183    | <div> <div>%</div> <div>58%</div> <div>33%</div> <div>5%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 183    |                  |
| 1   | G     | 183    |                  |
| 1   | H     | 183    |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | SGN  | A     | 1210 | -         | -        | -       | X                |
| 2   | SGN  | A     | 1212 | -         | -        | -       | X                |
| 2   | IDS  | A     | 1213 | X         | -        | -       | -                |
| 3   | SO4  | A     | 1215 | -         | -        | -       | X                |
| 3   | SO4  | C     | 1209 | -         | -        | X       | -                |
| 3   | SO4  | F     | 1216 | -         | -        | X       | -                |
| 4   | EPE  | F     | 1218 | -         | -        | -       | X                |
| 5   | SGN  | B     | 1210 | -         | -        | -       | X                |
| 6   | IDS  | B     | 1223 | X         | -        | -       | -                |
| 7   | SGN  | C     | 1212 | -         | -        | -       | X                |
| 8   | SGN  | G     | 1213 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11555 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 HEPATOCYTE GROWTH FACTOR.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 172      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1324  | 833 | 228 | 251 | 12 |         |         |       |
| 1   | B     | 172      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1339  | 843 | 231 | 253 | 12 |         |         |       |
| 1   | C     | 172      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1341  | 846 | 231 | 252 | 12 |         |         |       |
| 1   | D     | 172      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1305  | 821 | 223 | 249 | 12 |         |         |       |
| 1   | E     | 173      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1297  | 812 | 222 | 251 | 12 |         |         |       |
| 1   | F     | 173      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1331  | 836 | 231 | 252 | 12 |         |         |       |
| 1   | G     | 164      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1241  | 783 | 212 | 234 | 12 |         |         |       |
| 1   | H     | 171      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1299  | 814 | 224 | 249 | 12 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |
| A     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |
| B     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |
| B     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |
| C     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |
| C     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |
| D     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |
| D     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |
| E     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |
| E     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |
| F     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |
| F     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |
| G     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| G     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |
| H     | 29      | VAL      | ALA    | ENGINEERED MUTATION | UNP P14210 |
| H     | 72      | ASP      | ASN    | ENGINEERED MUTATION | UNP P14210 |

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 6        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 105   | 36 | 3 | 57 | 9 |         |         |

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



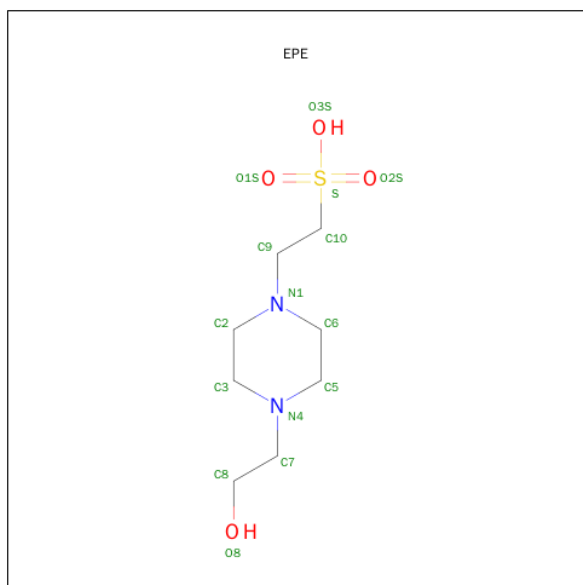
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |
| 4   | B     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |
| 4   | D     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |
| 4   | E     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |
| 4   | F     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |
| 4   | G     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |
| 4   | H     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

| Mol | Chain | Residues | Atoms |    |   |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|----|---------|---------|
| 5   | B     | 7        | Total | C  | N | O  | S  | 0       | 0       |
|     |       |          | 121   | 42 | 3 | 66 | 10 |         |         |

- Molecule 6 is a polymer of unknown type called SUGAR (8-MER).

| Mol | Chain | Residues | Atoms |    |   |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|----|---------|---------|
| 6   | B     | 8        | Total | C  | N | O  | S  | 0       | 0       |
|     |       |          | 140   | 48 | 4 | 76 | 12 |         |         |

- Molecule 7 is a polymer of unknown type called SUGAR (9-MER).

| Mol | Chain | Residues | Atoms |    |   |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|----|---------|---------|
| 7   | C     | 9        | Total | C  | N | O  | S  | 0       | 0       |
|     |       |          | 159   | 54 | 5 | 86 | 14 |         |         |

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 8   | F     | 6        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 105   | 36 | 3 | 57 | 9 |         |         |
| 8   | G     | 6        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 105   | 36 | 3 | 57 | 9 |         |         |

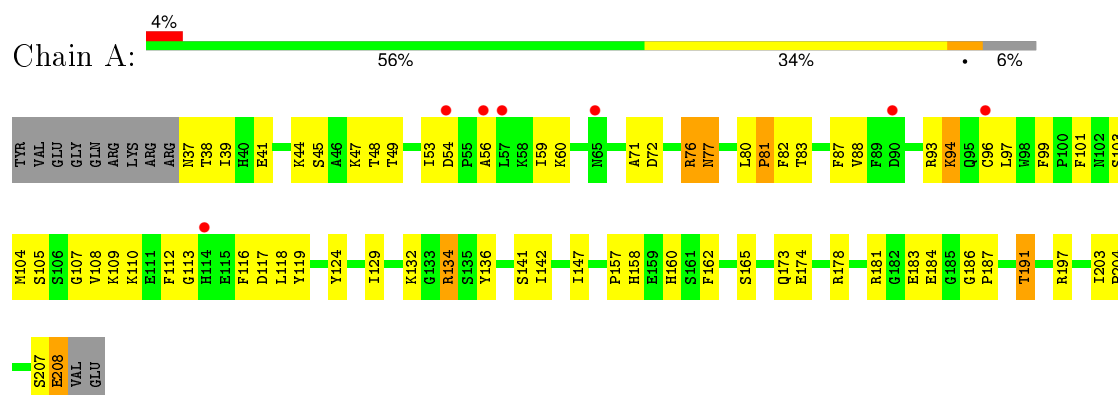
- Molecule 9 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | A     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 9   | B     | 34       | Total | O  | 0       | 0       |
|     |       |          | 34    | 34 |         |         |
| 9   | C     | 27       | Total | O  | 0       | 0       |
|     |       |          | 27    | 27 |         |         |
| 9   | D     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 9   | E     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 9   | F     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 9   | G     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 9   | H     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |

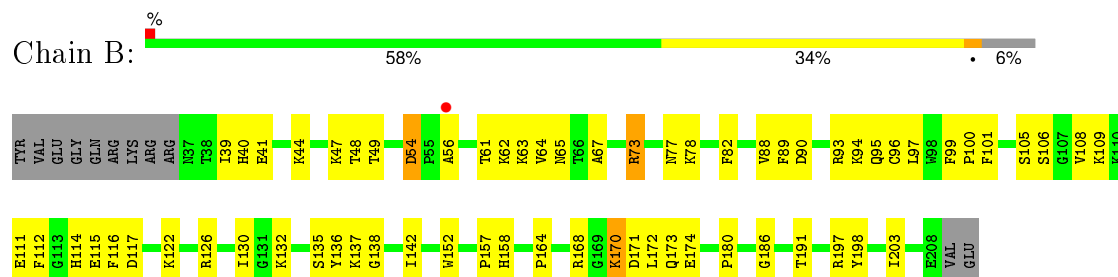
### 3 Residue-property plots

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

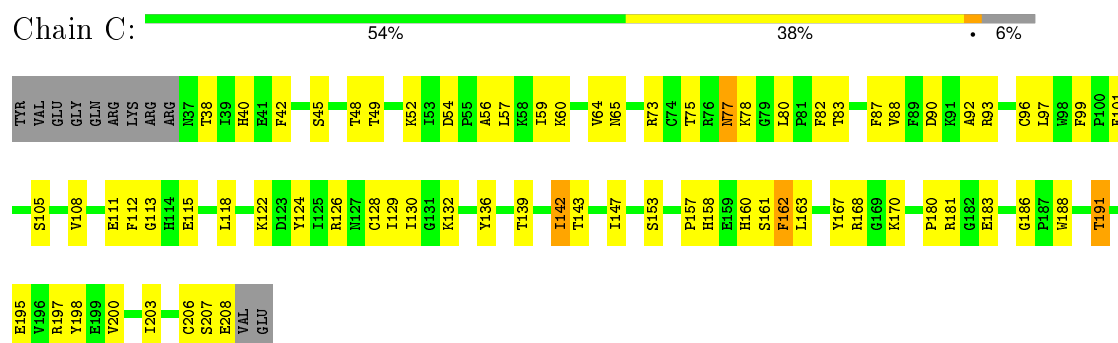
#### • Molecule 1: HEPATOCYTE GROWTH FACTOR



#### • Molecule 1: HEPATOCYTE GROWTH FACTOR



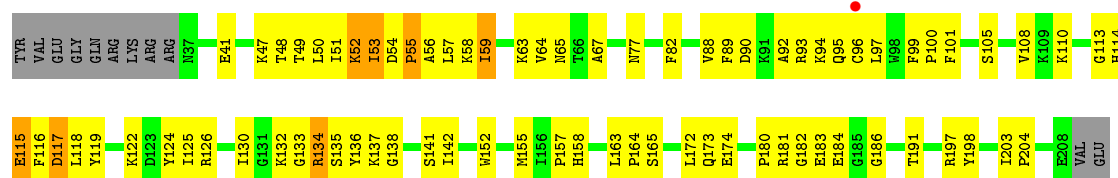
#### • Molecule 1: HEPATOCYTE GROWTH FACTOR



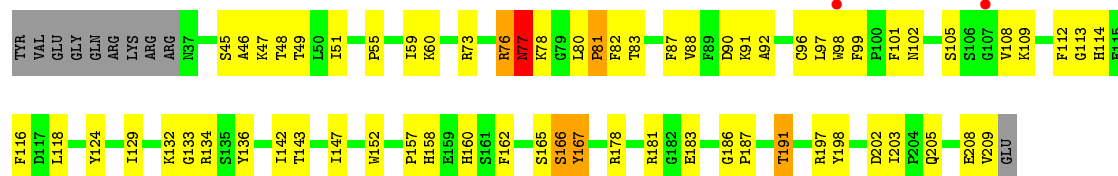
#### • Molecule 1: HEPATOCYTE GROWTH FACTOR



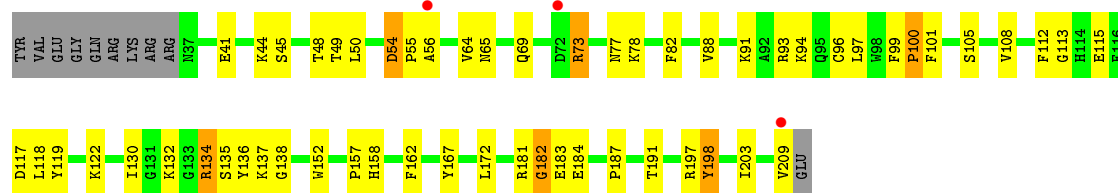




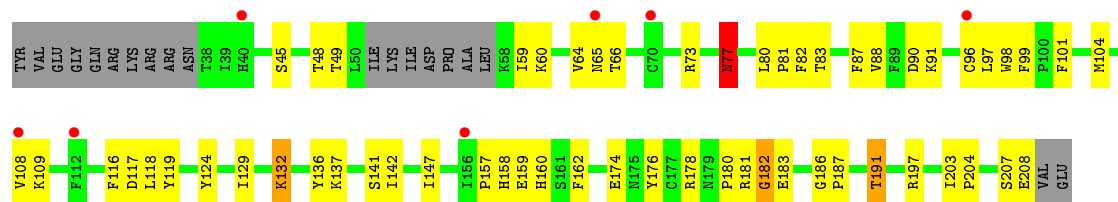
• Molecule 1: HEPATOCYTE GROWTH FACTOR



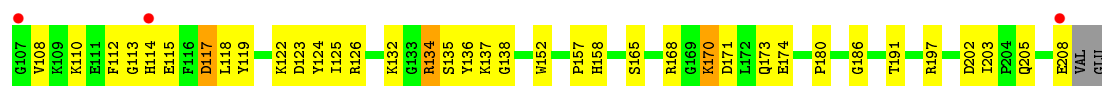
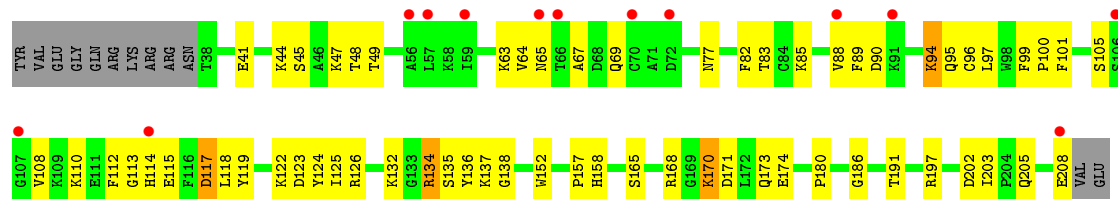
• Molecule 1: HEPATOCYTE GROWTH FACTOR



• Molecule 1: HEPATOCYTE GROWTH FACTOR



• Molecule 1: HEPATOCYTE GROWTH FACTOR



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 179.70Å 174.10Å 59.90Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 20.00 – 3.00<br>19.97 – 2.97                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.3 (20.00-3.00)<br>94.6 (19.97-2.97)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.26 (at 2.98Å)   | Xtriage          |
| Refinement program  | CNS 1.0   | Depositor        |
| R, $R_{free}$   | 0.254 , 0.295<br>0.268 , 0.298                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1824 reflections (4.98%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 59.5  | Xtriage          |
| Anisotropy  | 0.123   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 65.1   | EDS              |
| Estimated twinning fraction   | 0.005 for k,h,-l  | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Outliers  | 0 of 37652 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.88  | EDS              |
| Total number of atoms   | 11555   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 58.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, EPE, IDS, SGN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$ |
| 1   | A     | 0.45         | 0/1358      | 0.67        | 0/1835      |
| 1   | B     | 0.44         | 0/1374      | 0.63        | 0/1855      |
| 1   | C     | 0.50         | 0/1376      | 0.67        | 0/1859      |
| 1   | D     | 0.45         | 0/1338      | 0.63        | 0/1813      |
| 1   | E     | 0.45         | 0/1331      | 0.66        | 0/1808      |
| 1   | F     | 0.45         | 0/1365      | 0.66        | 0/1848      |
| 1   | G     | 0.38         | 0/1273      | 0.62        | 0/1724      |
| 1   | H     | 0.39         | 0/1334      | 0.59        | 0/1808      |
| All | All   | 0.44         | 0/10749     | 0.64        | 0/14550     |

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 |
|-----|-------|---------------------|---------------------|
| 2   | A     | 1                   | 0                   |
| 6   | B     | 1                   | 0                   |
| All | All   | 2                   | 0                   |

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 2   | A     | 1213 | IDS  | C4   |
| 6   | B     | 1223 | IDS  | C4   |

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1324  | 0        | 1221     | 73      | 0            |
| 1   | B     | 1339  | 0        | 1248     | 62      | 0            |
| 1   | C     | 1341  | 0        | 1257     | 71      | 0            |
| 1   | D     | 1305  | 0        | 1193     | 73      | 0            |
| 1   | E     | 1297  | 0        | 1140     | 72      | 0            |
| 1   | F     | 1331  | 0        | 1223     | 56      | 0            |
| 1   | G     | 1241  | 0        | 1121     | 55      | 0            |
| 1   | H     | 1299  | 0        | 1162     | 55      | 0            |
| 2   | A     | 105   | 0        | 39       | 0       | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 3   | B     | 5     | 0        | 0        | 0       | 0            |
| 3   | C     | 5     | 0        | 0        | 2       | 0            |
| 3   | D     | 5     | 0        | 0        | 1       | 0            |
| 3   | E     | 5     | 0        | 0        | 0       | 0            |
| 3   | F     | 10    | 0        | 0        | 2       | 0            |
| 3   | H     | 5     | 0        | 0        | 1       | 0            |
| 4   | A     | 15    | 0        | 17       | 1       | 0            |
| 4   | B     | 15    | 0        | 17       | 2       | 0            |
| 4   | C     | 15    | 0        | 17       | 3       | 0            |
| 4   | D     | 15    | 0        | 17       | 1       | 0            |
| 4   | E     | 15    | 0        | 17       | 1       | 0            |
| 4   | F     | 15    | 0        | 17       | 1       | 0            |
| 4   | G     | 15    | 0        | 17       | 0       | 0            |
| 4   | H     | 15    | 0        | 17       | 0       | 0            |
| 5   | B     | 121   | 0        | 44       | 1       | 0            |
| 6   | B     | 140   | 0        | 52       | 3       | 0            |
| 7   | C     | 159   | 0        | 61       | 2       | 0            |
| 8   | F     | 105   | 0        | 40       | 1       | 0            |
| 8   | G     | 105   | 0        | 40       | 0       | 0            |
| 9   | A     | 21    | 0        | 0        | 0       | 0            |
| 9   | B     | 34    | 0        | 0        | 5       | 0            |
| 9   | C     | 27    | 0        | 0        | 6       | 0            |
| 9   | D     | 22    | 0        | 0        | 7       | 0            |
| 9   | E     | 29    | 0        | 0        | 7       | 0            |
| 9   | F     | 20    | 0        | 0        | 3       | 0            |
| 9   | G     | 17    | 0        | 0        | 3       | 0            |
| 9   | H     | 13    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 11555 | 0        | 9977     | 513     | 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 24.

All (513) 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:181:ARG:NH2  | 1:H:165:SER:HB3  | 1.63                     | 1.12              |
| 1:D:52:LYS:H     | 1:D:52:LYS:HD3   | 1.22                     | 1.01              |
| 1:A:134:ARG:HD2  | 1:A:134:ARG:H    | 1.26                     | 0.98              |
| 1:F:64:VAL:HG13  | 1:F:69:GLN:OE1   | 1.64                     | 0.96              |
| 1:G:132:LYS:H    | 1:G:132:LYS:HD2  | 1.31                     | 0.96              |
| 1:H:134:ARG:HD2  | 1:H:134:ARG:H    | 1.32                     | 0.94              |
| 1:D:97:LEU:HD23  | 9:D:2001:HOH:O   | 1.69                     | 0.92              |
| 1:G:207:SER:O    | 1:G:208:GLU:HB2  | 1.67                     | 0.91              |
| 1:C:93:ARG:HH11  | 1:C:93:ARG:HG3   | 1.35                     | 0.90              |
| 1:C:122:LYS:HE2  | 1:C:139:THR:HG21 | 1.54                     | 0.89              |
| 1:E:181:ARG:HH21 | 1:H:165:SER:HB3  | 1.36                     | 0.88              |
| 1:F:134:ARG:HD2  | 1:F:134:ARG:H    | 1.40                     | 0.87              |
| 1:H:170:LYS:HG2  | 1:H:180:PRO:HA   | 1.57                     | 0.86              |
| 1:E:101:PHE:HB2  | 1:E:105:SER:OG   | 1.76                     | 0.85              |
| 1:A:103:SER:HB2  | 1:A:110:LYS:HE2  | 1.59                     | 0.82              |
| 1:A:207:SER:O    | 1:A:208:GLU:HB2  | 1.79                     | 0.82              |
| 1:A:72:ASP:OD1   | 1:A:76:ARG:HD2   | 1.79                     | 0.82              |
| 1:F:132:LYS:HB2  | 1:F:134:ARG:HE   | 1.44                     | 0.81              |
| 1:H:132:LYS:HB2  | 1:H:134:ARG:HE   | 1.46                     | 0.80              |
| 1:E:181:ARG:HH21 | 1:H:165:SER:CB   | 1.94                     | 0.80              |
| 1:C:38:THR:HG21  | 1:C:75:THR:OG1   | 1.81                     | 0.80              |
| 1:F:73:ARG:HH11  | 1:F:73:ARG:HG3   | 1.48                     | 0.79              |
| 4:B:1225:EPE:H21 | 9:B:2029:HOH:O   | 1.86                     | 0.76              |
| 1:G:66:THR:HB    | 9:G:2002:HOH:O   | 1.85                     | 0.75              |
| 1:B:88:VAL:HG23  | 1:B:99:PHE:HE1   | 1.51                     | 0.75              |
| 1:A:160:HIS:HD2  | 1:A:162:PHE:H    | 1.32                     | 0.75              |
| 1:D:52:LYS:HD3   | 1:D:52:LYS:N     | 2.00                     | 0.74              |
| 1:D:181:ARG:HB2  | 1:D:183:GLU:HG3  | 1.70                     | 0.74              |
| 1:A:37:ASN:O     | 1:A:39:ILE:N     | 2.21                     | 0.74              |
| 1:B:73:ARG:NH2   | 6:B:1222:SGN:H62 | 2.01                     | 0.74              |
| 1:C:183:GLU:OE1  | 4:C:1219:EPE:H51 | 1.87                     | 0.74              |
| 1:B:126:ARG:NH1  | 1:B:130:ILE:HD11 | 2.02                     | 0.73              |
| 1:F:64:VAL:HG11  | 1:F:69:GLN:HB2   | 1.69                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:132:LYS:HA   | 9:G:2008:HOH:O   | 1.86                     | 0.73              |
| 1:E:59:ILE:HG22  | 1:E:60:LYS:N     | 2.04                     | 0.72              |
| 1:A:96:CYS:C     | 1:A:97:LEU:HD12  | 2.09                     | 0.72              |
| 1:A:160:HIS:CD2  | 1:A:162:PHE:H    | 2.06                     | 0.72              |
| 1:B:73:ARG:HG3   | 1:B:73:ARG:HH11  | 1.53                     | 0.72              |
| 1:B:54:ASP:HB3   | 9:B:2007:HOH:O   | 1.89                     | 0.71              |
| 1:G:160:HIS:HD2  | 1:G:162:PHE:H    | 1.36                     | 0.71              |
| 1:C:93:ARG:HG3   | 1:C:93:ARG:NH1   | 2.00                     | 0.71              |
| 1:B:170:LYS:HG2  | 1:B:180:PRO:HA   | 1.71                     | 0.71              |
| 1:D:130:ILE:N    | 3:D:1209:SO4:O2  | 2.22                     | 0.70              |
| 1:H:64:VAL:HG13  | 1:H:69:GLN:OE1   | 1.92                     | 0.70              |
| 1:E:96:CYS:C     | 1:E:97:LEU:HD12  | 2.13                     | 0.69              |
| 1:E:158:HIS:NE2  | 1:E:197:ARG:HA   | 2.06                     | 0.69              |
| 1:E:181:ARG:HH22 | 1:H:165:SER:HB3  | 1.55                     | 0.69              |
| 1:G:132:LYS:N    | 1:G:132:LYS:HD2  | 2.07                     | 0.69              |
| 1:A:158:HIS:NE2  | 1:A:197:ARG:HA   | 2.08                     | 0.69              |
| 1:C:96:CYS:C     | 1:C:97:LEU:HD12  | 2.13                     | 0.69              |
| 1:G:96:CYS:C     | 1:G:97:LEU:HD12  | 2.13                     | 0.68              |
| 1:A:59:ILE:HG22  | 1:A:60:LYS:N     | 2.09                     | 0.68              |
| 1:C:59:ILE:HG22  | 1:C:60:LYS:N     | 2.09                     | 0.67              |
| 1:E:205:GLN:HG2  | 9:E:2028:HOH:O   | 1.94                     | 0.67              |
| 1:C:158:HIS:NE2  | 1:C:197:ARG:HA   | 2.10                     | 0.66              |
| 1:E:181:ARG:NH2  | 1:H:165:SER:CB   | 2.48                     | 0.66              |
| 1:A:101:PHE:HB2  | 1:A:105:SER:CB   | 2.26                     | 0.66              |
| 1:A:93:ARG:O     | 1:A:94:LYS:HB2   | 1.95                     | 0.66              |
| 1:B:73:ARG:HH22  | 6:B:1222:SGN:H62 | 1.60                     | 0.66              |
| 1:G:160:HIS:CD2  | 1:G:162:PHE:H    | 2.13                     | 0.66              |
| 1:G:88:VAL:HG23  | 1:G:99:PHE:HE2   | 1.60                     | 0.65              |
| 1:G:45:SER:HB2   | 1:G:118:LEU:HB3  | 1.77                     | 0.65              |
| 1:A:134:ARG:HD2  | 1:A:134:ARG:N    | 2.06                     | 0.65              |
| 1:H:63:LYS:O     | 1:H:64:VAL:HG23  | 1.97                     | 0.65              |
| 1:D:59:ILE:HG22  | 1:D:59:ILE:O     | 1.97                     | 0.65              |
| 1:F:105:SER:O    | 1:F:108:VAL:HG22 | 1.97                     | 0.65              |
| 1:A:132:LYS:HB2  | 1:A:134:ARG:NE   | 2.12                     | 0.65              |
| 1:H:105:SER:O    | 1:H:108:VAL:HG22 | 1.97                     | 0.65              |
| 1:B:111:GLU:CD   | 1:B:112:PHE:H    | 1.99                     | 0.65              |
| 1:B:105:SER:O    | 1:B:108:VAL:HG22 | 1.98                     | 0.64              |
| 7:C:1213:IDS:H2  | 9:C:2025:HOH:O   | 1.97                     | 0.64              |
| 1:E:88:VAL:HG23  | 1:E:99:PHE:HE2   | 1.61                     | 0.64              |
| 1:A:45:SER:HB2   | 1:A:118:LEU:HB3  | 1.78                     | 0.64              |
| 1:A:141:SER:O    | 1:A:142:ILE:HD12 | 1.98                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:132:LYS:HB2  | 1:H:134:ARG:NE   | 2.12                     | 0.64              |
| 1:G:59:ILE:HG22  | 1:G:60:LYS:N     | 2.13                     | 0.63              |
| 1:C:88:VAL:HG23  | 1:C:99:PHE:HE2   | 1.63                     | 0.63              |
| 1:D:47:LYS:N     | 1:D:116:PHE:O    | 2.31                     | 0.63              |
| 1:A:88:VAL:HG23  | 1:A:99:PHE:HE2   | 1.63                     | 0.63              |
| 1:C:45:SER:HB2   | 1:C:118:LEU:HB3  | 1.81                     | 0.63              |
| 1:G:158:HIS:NE2  | 1:G:197:ARG:HA   | 2.13                     | 0.62              |
| 1:H:170:LYS:HE3  | 1:H:170:LYS:N    | 2.14                     | 0.62              |
| 1:E:132:LYS:O    | 1:E:186:GLY:HA2  | 1.99                     | 0.62              |
| 1:D:105:SER:O    | 1:D:108:VAL:HG22 | 1.99                     | 0.62              |
| 1:D:184:GLU:O    | 4:D:1210:EPE:H81 | 1.99                     | 0.62              |
| 1:D:64:VAL:CG1   | 1:D:65:ASN:N     | 2.63                     | 0.62              |
| 1:D:63:LYS:O     | 1:D:64:VAL:HG23  | 1.99                     | 0.62              |
| 1:E:45:SER:HB2   | 1:E:118:LEU:HB3  | 1.80                     | 0.61              |
| 1:E:96:CYS:HB3   | 9:E:2008:HOH:O   | 1.99                     | 0.61              |
| 1:D:158:HIS:CE1  | 1:D:197:ARG:HA   | 2.35                     | 0.61              |
| 1:G:207:SER:O    | 1:G:208:GLU:CB   | 2.43                     | 0.61              |
| 1:H:64:VAL:HG11  | 1:H:69:GLN:HB2   | 1.83                     | 0.61              |
| 1:E:114:HIS:HA   | 9:E:2010:HOH:O   | 2.00                     | 0.61              |
| 1:A:184:GLU:O    | 4:A:1216:EPE:H81 | 1.99                     | 0.61              |
| 1:C:170:LYS:HD2  | 1:C:180:PRO:HA   | 1.82                     | 0.61              |
| 1:E:152:TRP:N    | 9:E:2018:HOH:O   | 2.33                     | 0.61              |
| 1:E:47:LYS:HA    | 1:E:113:GLY:O    | 2.01                     | 0.61              |
| 1:B:64:VAL:CG1   | 1:B:65:ASN:N     | 2.64                     | 0.61              |
| 1:E:208:GLU:O    | 1:E:209:VAL:HG23 | 2.01                     | 0.60              |
| 1:C:160:HIS:HD2  | 1:C:162:PHE:HB2  | 1.66                     | 0.60              |
| 1:B:106:SER:HA   | 9:B:2006:HOH:O   | 2.01                     | 0.60              |
| 1:G:181:ARG:HB2  | 1:G:183:GLU:HG3  | 1.83                     | 0.60              |
| 1:G:132:LYS:H    | 1:G:132:LYS:CD   | 2.11                     | 0.60              |
| 1:C:130:ILE:N    | 3:C:1209:SO4:O1  | 2.34                     | 0.60              |
| 1:C:126:ARG:HD3  | 1:C:206:CYS:SG   | 2.40                     | 0.60              |
| 1:D:52:LYS:H     | 1:D:52:LYS:CD    | 1.99                     | 0.60              |
| 1:H:88:VAL:HG23  | 1:H:99:PHE:HE2   | 1.64                     | 0.60              |
| 1:B:88:VAL:HG23  | 1:B:99:PHE:CE1   | 2.35                     | 0.60              |
| 1:A:96:CYS:O     | 1:A:97:LEU:HD12  | 2.01                     | 0.60              |
| 1:F:198:TYR:CD1  | 4:F:1218:EPE:H22 | 2.36                     | 0.60              |
| 1:G:160:HIS:CD2  | 1:G:162:PHE:HB2  | 2.37                     | 0.60              |
| 4:C:1219:EPE:H61 | 9:C:2019:HOH:O   | 2.03                     | 0.59              |
| 1:E:59:ILE:CG2   | 1:E:60:LYS:N     | 2.65                     | 0.59              |
| 1:H:170:LYS:HE3  | 1:H:170:LYS:CA   | 2.32                     | 0.59              |
| 1:B:126:ARG:NH1  | 1:B:130:ILE:CD1  | 2.66                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:48:THR:HG22  | 1:G:49:THR:N     | 2.18                     | 0.59              |
| 1:C:198:TYR:CD1  | 1:C:198:TYR:C    | 2.77                     | 0.58              |
| 1:A:132:LYS:O    | 1:A:186:GLY:HA2  | 2.03                     | 0.58              |
| 1:F:73:ARG:NH1   | 1:F:73:ARG:HG3   | 2.17                     | 0.58              |
| 1:F:88:VAL:HG23  | 1:F:99:PHE:CE2   | 2.38                     | 0.58              |
| 1:D:48:THR:O     | 1:D:116:PHE:HB3  | 2.03                     | 0.58              |
| 1:A:41:GLU:HG2   | 1:B:41:GLU:HG2   | 1.85                     | 0.58              |
| 1:E:102:ASN:N    | 1:E:105:SER:OG   | 2.35                     | 0.58              |
| 1:A:39:ILE:HD11  | 1:A:119:TYR:CE2  | 2.39                     | 0.58              |
| 1:B:126:ARG:HH12 | 1:B:130:ILE:CD1  | 2.16                     | 0.58              |
| 1:G:132:LYS:O    | 1:G:186:GLY:HA2  | 2.03                     | 0.58              |
| 1:G:160:HIS:HD2  | 1:G:162:PHE:HB2  | 1.68                     | 0.58              |
| 1:D:58:LYS:N     | 9:D:2003:HOH:O   | 2.36                     | 0.58              |
| 1:H:158:HIS:CE1  | 1:H:197:ARG:HA   | 2.38                     | 0.58              |
| 1:D:96:CYS:C     | 1:D:97:LEU:HD12  | 2.24                     | 0.58              |
| 1:B:126:ARG:HH12 | 1:B:130:ILE:HD11 | 1.68                     | 0.58              |
| 1:H:64:VAL:CG1   | 1:H:65:ASN:N     | 2.67                     | 0.58              |
| 1:F:88:VAL:HG23  | 1:F:99:PHE:HE2   | 1.69                     | 0.58              |
| 1:F:158:HIS:CE1  | 1:F:197:ARG:HA   | 2.38                     | 0.58              |
| 1:D:117:ASP:HB3  | 1:D:119:TYR:CE1  | 2.39                     | 0.58              |
| 1:A:118:LEU:HD12 | 1:A:119:TYR:H    | 1.69                     | 0.58              |
| 1:G:141:SER:C    | 1:G:142:ILE:HD12 | 2.25                     | 0.58              |
| 1:A:117:ASP:HB3  | 1:A:119:TYR:HE1  | 1.69                     | 0.57              |
| 1:G:141:SER:O    | 1:G:142:ILE:HD12 | 2.04                     | 0.57              |
| 1:B:96:CYS:C     | 1:B:97:LEU:HD12  | 2.25                     | 0.57              |
| 1:B:158:HIS:CE1  | 1:B:197:ARG:HA   | 2.39                     | 0.57              |
| 1:C:48:THR:HG22  | 1:C:49:THR:N     | 2.19                     | 0.57              |
| 1:C:200:VAL:HG13 | 9:C:2022:HOH:O   | 2.04                     | 0.57              |
| 1:F:64:VAL:CG1   | 1:F:65:ASN:N     | 2.67                     | 0.57              |
| 1:H:157:PRO:HG2  | 1:H:158:HIS:CD2  | 2.40                     | 0.57              |
| 1:A:48:THR:HG22  | 1:A:49:THR:N     | 2.20                     | 0.57              |
| 1:F:122:LYS:HE3  | 9:F:2004:HOH:O   | 2.05                     | 0.57              |
| 1:A:39:ILE:HD11  | 1:A:119:TYR:HE2  | 1.68                     | 0.57              |
| 1:D:88:VAL:HG23  | 1:D:99:PHE:HE2   | 1.69                     | 0.57              |
| 1:G:73:ARG:HD3   | 1:G:98:TRP:CH2   | 2.40                     | 0.56              |
| 1:E:101:PHE:HB2  | 1:E:105:SER:CB   | 2.35                     | 0.56              |
| 1:F:50:LEU:HD22  | 1:F:99:PHE:CD2   | 2.41                     | 0.56              |
| 1:G:73:ARG:HD3   | 1:G:98:TRP:CZ2   | 2.39                     | 0.56              |
| 1:D:41:GLU:O     | 1:D:122:LYS:HG3  | 2.06                     | 0.56              |
| 1:H:64:VAL:HG13  | 1:H:69:GLN:CD    | 2.26                     | 0.56              |
| 1:F:134:ARG:CD   | 1:F:134:ARG:H    | 2.11                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:165:SER:C    | 1:E:167:TYR:H    | 2.09                     | 0.56              |
| 1:A:44:LYS:HE3   | 1:A:119:TYR:OH   | 2.04                     | 0.56              |
| 1:E:208:GLU:O    | 1:E:209:VAL:HB   | 2.04                     | 0.56              |
| 1:D:50:LEU:C     | 1:D:51:ILE:HD12  | 2.25                     | 0.56              |
| 1:C:59:ILE:CG2   | 1:C:60:LYS:N     | 2.69                     | 0.56              |
| 1:C:83:THR:HG21  | 1:C:124:TYR:OH   | 2.06                     | 0.56              |
| 1:H:47:LYS:HG3   | 1:H:114:HIS:HA   | 1.88                     | 0.56              |
| 1:E:48:THR:HG22  | 1:E:49:THR:N     | 2.21                     | 0.56              |
| 1:E:208:GLU:O    | 1:E:209:VAL:CB   | 2.52                     | 0.55              |
| 1:F:157:PRO:HG2  | 1:F:158:HIS:CD2  | 2.41                     | 0.55              |
| 1:D:50:LEU:CD1   | 1:D:118:LEU:HD22 | 2.36                     | 0.55              |
| 1:F:41:GLU:O     | 1:F:122:LYS:HG3  | 2.06                     | 0.55              |
| 1:B:73:ARG:NH1   | 1:B:73:ARG:HG3   | 2.21                     | 0.55              |
| 1:D:157:PRO:HG2  | 1:D:158:HIS:CD2  | 2.41                     | 0.55              |
| 1:B:41:GLU:O     | 1:B:122:LYS:HG3  | 2.05                     | 0.55              |
| 1:C:105:SER:O    | 1:C:108:VAL:HB   | 2.06                     | 0.55              |
| 1:G:117:ASP:HB3  | 1:G:119:TYR:CE1  | 2.41                     | 0.55              |
| 1:C:207:SER:O    | 1:C:208:GLU:CB   | 2.54                     | 0.55              |
| 1:D:53:ILE:O     | 1:D:54:ASP:C     | 2.45                     | 0.55              |
| 1:F:96:CYS:C     | 1:F:97:LEU:HD12  | 2.27                     | 0.55              |
| 1:C:122:LYS:HD3  | 1:C:139:THR:OG1  | 2.06                     | 0.55              |
| 1:A:83:THR:HG21  | 1:A:124:TYR:OH   | 2.06                     | 0.55              |
| 1:E:158:HIS:CD2  | 1:E:197:ARG:HA   | 2.41                     | 0.55              |
| 1:C:160:HIS:CD2  | 1:C:162:PHE:HB2  | 2.42                     | 0.55              |
| 1:F:45:SER:HB2   | 1:F:118:LEU:HB3  | 1.89                     | 0.55              |
| 1:B:93:ARG:HH11  | 1:B:93:ARG:HG3   | 1.71                     | 0.55              |
| 1:C:38:THR:CG2   | 1:C:75:THR:OG1   | 2.54                     | 0.54              |
| 1:C:207:SER:O    | 1:C:208:GLU:HB3  | 2.08                     | 0.54              |
| 1:G:90:ASP:OD2   | 1:G:116:PHE:HE1  | 1.90                     | 0.54              |
| 1:C:158:HIS:CD2  | 1:C:197:ARG:HA   | 2.42                     | 0.54              |
| 1:G:147:ILE:HG21 | 1:G:191:THR:HB   | 1.90                     | 0.54              |
| 1:F:136:TYR:CZ   | 1:F:138:GLY:HA3  | 2.43                     | 0.54              |
| 1:E:147:ILE:HG21 | 1:E:191:THR:HB   | 1.90                     | 0.54              |
| 1:B:61:THR:O     | 1:B:62:LYS:HB2   | 2.08                     | 0.54              |
| 1:A:162:PHE:CE1  | 1:A:181:ARG:HD2  | 2.42                     | 0.54              |
| 1:H:41:GLU:O     | 1:H:122:LYS:HG3  | 2.08                     | 0.54              |
| 1:B:170:LYS:CG   | 1:B:180:PRO:HA   | 2.38                     | 0.53              |
| 1:A:59:ILE:CG2   | 1:A:60:LYS:N     | 2.70                     | 0.53              |
| 1:H:96:CYS:C     | 1:H:97:LEU:HD12  | 2.28                     | 0.53              |
| 1:D:134:ARG:HD2  | 9:D:2008:HOH:O   | 2.07                     | 0.53              |
| 1:D:49:THR:O     | 1:D:110:LYS:HA   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:83:THR:HG21  | 1:G:124:TYR:OH   | 2.08                     | 0.53              |
| 1:C:161:SER:O    | 1:C:163:LEU:N    | 2.41                     | 0.53              |
| 1:A:162:PHE:HE1  | 1:A:181:ARG:HD2  | 1.73                     | 0.53              |
| 1:F:93:ARG:O     | 1:F:94:LYS:HB2   | 2.08                     | 0.53              |
| 1:A:158:HIS:CD2  | 1:A:197:ARG:HA   | 2.43                     | 0.53              |
| 1:H:135:SER:O    | 1:H:137:LYS:HG3  | 2.09                     | 0.53              |
| 1:A:118:LEU:HD12 | 1:A:119:TYR:N    | 2.23                     | 0.53              |
| 1:C:147:ILE:HG21 | 1:C:191:THR:HB   | 1.90                     | 0.53              |
| 1:B:82:PHE:CD1   | 1:B:100:PRO:HB3  | 2.43                     | 0.53              |
| 1:B:198:TYR:CE2  | 4:B:1225:EPE:H52 | 2.44                     | 0.53              |
| 1:E:59:ILE:HG22  | 1:E:60:LYS:H     | 1.74                     | 0.53              |
| 1:E:76:ARG:O     | 1:E:78:LYS:N     | 2.42                     | 0.53              |
| 1:G:160:HIS:HD2  | 1:G:162:PHE:N    | 2.06                     | 0.52              |
| 1:E:96:CYS:O     | 1:E:97:LEU:HD12  | 2.09                     | 0.52              |
| 1:F:44:LYS:HD3   | 1:F:119:TYR:CE2  | 2.44                     | 0.52              |
| 1:E:59:ILE:CG2   | 1:E:60:LYS:H     | 2.22                     | 0.52              |
| 1:A:108:VAL:HG12 | 1:A:109:LYS:N    | 2.24                     | 0.52              |
| 1:H:90:ASP:OD1   | 1:H:115:GLU:OE1  | 2.28                     | 0.52              |
| 1:C:132:LYS:O    | 1:C:186:GLY:HA2  | 2.10                     | 0.52              |
| 1:D:135:SER:O    | 1:D:137:LYS:HG3  | 2.08                     | 0.52              |
| 1:F:73:ARG:HH22  | 8:F:1214:SGN:H62 | 1.73                     | 0.52              |
| 1:B:97:LEU:HB3   | 1:B:99:PHE:CZ    | 2.45                     | 0.52              |
| 1:D:64:VAL:HG12  | 1:D:65:ASN:N     | 2.24                     | 0.52              |
| 1:H:112:PHE:CD1  | 1:H:113:GLY:N    | 2.76                     | 0.52              |
| 1:A:77:ASN:O     | 1:A:77:ASN:ND2   | 2.42                     | 0.52              |
| 1:G:59:ILE:CG2   | 1:G:60:LYS:N     | 2.73                     | 0.52              |
| 1:B:82:PHE:CG    | 1:B:100:PRO:HB3  | 2.45                     | 0.51              |
| 1:C:73:ARG:NE    | 1:C:78:LYS:O     | 2.43                     | 0.51              |
| 1:F:132:LYS:HB2  | 1:F:134:ARG:NE   | 2.20                     | 0.51              |
| 1:A:160:HIS:CD2  | 1:A:162:PHE:HB2  | 2.45                     | 0.51              |
| 1:B:73:ARG:NE    | 1:B:78:LYS:O     | 2.43                     | 0.51              |
| 1:B:54:ASP:OD1   | 1:B:56:ALA:CB    | 2.58                     | 0.51              |
| 1:B:135:SER:O    | 1:B:137:LYS:HG3  | 2.10                     | 0.51              |
| 1:F:54:ASP:O     | 1:F:56:ALA:N     | 2.44                     | 0.51              |
| 1:D:117:ASP:HB3  | 1:D:119:TYR:HE1  | 1.75                     | 0.51              |
| 1:B:136:TYR:CZ   | 1:B:138:GLY:HA3  | 2.45                     | 0.51              |
| 1:D:132:LYS:O    | 1:D:186:GLY:HA2  | 2.11                     | 0.51              |
| 1:G:96:CYS:O     | 1:G:97:LEU:HD12  | 2.09                     | 0.51              |
| 1:D:155:MET:CE   | 1:D:163:LEU:HD21 | 2.40                     | 0.51              |
| 1:H:168:ARG:O    | 1:H:170:LYS:NZ   | 2.43                     | 0.51              |
| 1:B:48:THR:O     | 1:B:116:PHE:HB3  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:38:THR:HG21  | 1:C:75:THR:CB   | 2.40                     | 0.51              |
| 1:D:118:LEU:HD12 | 1:D:119:TYR:H   | 1.76                     | 0.51              |
| 1:H:171:ASP:HA   | 3:H:1209:SO4:O1 | 2.10                     | 0.51              |
| 1:H:205:GLN:HB2  | 1:H:208:GLU:HG2 | 1.94                     | 0.50              |
| 1:G:158:HIS:CD2  | 1:G:197:ARG:HA  | 2.45                     | 0.50              |
| 1:H:173:GLN:O    | 1:H:174:GLU:C   | 2.49                     | 0.50              |
| 1:C:77:ASN:ND2   | 1:C:77:ASN:O    | 2.44                     | 0.50              |
| 1:B:157:PRO:HG2  | 1:B:158:HIS:CD2 | 2.45                     | 0.50              |
| 1:C:153:SER:HA   | 9:C:2014:HOH:O  | 2.10                     | 0.50              |
| 1:H:136:TYR:CZ   | 1:H:138:GLY:HA3 | 2.47                     | 0.50              |
| 1:H:82:PHE:CD1   | 1:H:100:PRO:HB3 | 2.47                     | 0.50              |
| 1:A:54:ASP:OD1   | 1:A:56:ALA:HB3  | 2.12                     | 0.50              |
| 1:D:164:PRO:HD2  | 9:D:2015:HOH:O  | 2.10                     | 0.50              |
| 1:C:96:CYS:O     | 1:C:97:LEU:HD12 | 2.10                     | 0.50              |
| 1:B:64:VAL:HG12  | 1:B:65:ASN:N    | 2.26                     | 0.50              |
| 1:E:208:GLU:O    | 1:E:209:VAL:CG2 | 2.59                     | 0.50              |
| 1:F:88:VAL:HG13  | 1:F:117:ASP:O   | 2.12                     | 0.50              |
| 1:E:142:ILE:HG22 | 1:E:143:THR:O   | 2.12                     | 0.50              |
| 1:D:58:LYS:CB    | 9:D:2003:HOH:O  | 2.60                     | 0.50              |
| 1:H:45:SER:HB2   | 1:H:118:LEU:HB3 | 1.92                     | 0.50              |
| 1:G:132:LYS:N    | 1:G:132:LYS:CD  | 2.72                     | 0.49              |
| 1:C:49:THR:HG22  | 1:C:111:GLU:O   | 2.11                     | 0.49              |
| 1:B:109:LYS:HA   | 9:B:2008:HOH:O  | 2.11                     | 0.49              |
| 1:H:132:LYS:O    | 1:H:186:GLY:HA2 | 2.12                     | 0.49              |
| 1:E:166:SER:O    | 1:E:167:TYR:CG  | 2.65                     | 0.49              |
| 1:F:134:ARG:HD2  | 1:F:134:ARG:N   | 2.20                     | 0.49              |
| 1:B:54:ASP:OD1   | 1:B:56:ALA:HB3  | 2.13                     | 0.49              |
| 1:B:93:ARG:NH1   | 1:B:115:GLU:OE1 | 2.45                     | 0.49              |
| 1:F:91:LYS:N     | 1:F:115:GLU:O   | 2.44                     | 0.49              |
| 1:A:132:LYS:HB2  | 1:A:134:ARG:CZ  | 2.42                     | 0.49              |
| 1:C:93:ARG:CG    | 1:C:93:ARG:HH11 | 2.14                     | 0.49              |
| 1:D:63:LYS:HA    | 1:D:95:GLN:HB2  | 1.94                     | 0.49              |
| 1:A:97:LEU:HB3   | 1:A:99:PHE:CZ   | 2.48                     | 0.49              |
| 1:F:187:PRO:O    | 9:F:2016:HOH:O  | 2.20                     | 0.49              |
| 1:F:181:ARG:O    | 1:F:182:GLY:C   | 2.50                     | 0.49              |
| 1:A:160:HIS:HD2  | 1:A:162:PHE:HB2 | 1.77                     | 0.49              |
| 1:H:64:VAL:HG12  | 1:H:65:ASN:N    | 2.28                     | 0.49              |
| 1:B:171:ASP:OD1  | 1:B:173:GLN:HG2 | 2.13                     | 0.49              |
| 1:C:126:ARG:HG2  | 1:C:128:CYS:H   | 1.78                     | 0.49              |
| 1:B:173:GLN:O    | 1:B:174:GLU:C   | 2.51                     | 0.49              |
| 1:D:90:ASP:OD1   | 1:D:93:ARG:N    | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:82:PHE:CG    | 1:H:100:PRO:HB3  | 2.48                     | 0.48              |
| 1:F:73:ARG:NE    | 1:F:78:LYS:O     | 2.45                     | 0.48              |
| 1:A:39:ILE:CG1   | 1:A:119:TYR:HE2  | 2.26                     | 0.48              |
| 1:B:132:LYS:O    | 1:B:186:GLY:HA2  | 2.14                     | 0.48              |
| 1:A:99:PHE:HB3   | 1:A:101:PHE:CZ   | 2.49                     | 0.48              |
| 1:D:64:VAL:O     | 1:D:94:LYS:O     | 2.31                     | 0.48              |
| 1:C:168:ARG:C    | 1:C:170:LYS:H    | 2.17                     | 0.48              |
| 1:E:162:PHE:HE1  | 1:E:181:ARG:HD2  | 1.79                     | 0.48              |
| 1:E:83:THR:HG21  | 1:E:124:TYR:OH   | 2.14                     | 0.48              |
| 1:D:82:PHE:CD1   | 1:D:100:PRO:HB3  | 2.48                     | 0.48              |
| 1:D:52:LYS:CD    | 1:D:52:LYS:N     | 2.69                     | 0.48              |
| 1:E:97:LEU:HB3   | 1:E:99:PHE:CZ    | 2.49                     | 0.48              |
| 1:F:135:SER:O    | 1:F:137:LYS:HG3  | 2.13                     | 0.48              |
| 1:D:50:LEU:HD11  | 1:D:118:LEU:HD22 | 1.94                     | 0.48              |
| 1:C:129:ILE:HG22 | 1:C:136:TYR:HB2  | 1.96                     | 0.48              |
| 1:C:54:ASP:HB3   | 1:C:57:LEU:CD1   | 2.43                     | 0.48              |
| 1:A:207:SER:O    | 1:A:208:GLU:CB   | 2.59                     | 0.48              |
| 1:G:97:LEU:HB3   | 1:G:99:PHE:CZ    | 2.49                     | 0.48              |
| 1:G:157:PRO:HG2  | 1:G:158:HIS:CE1  | 2.49                     | 0.47              |
| 1:B:101:PHE:CE1  | 1:B:108:VAL:HG11 | 2.49                     | 0.47              |
| 1:D:113:GLY:C    | 1:D:115:GLU:H    | 2.18                     | 0.47              |
| 1:F:122:LYS:CE   | 9:F:2004:HOH:O   | 2.62                     | 0.47              |
| 1:D:136:TYR:CZ   | 1:D:203:ILE:HD13 | 2.49                     | 0.47              |
| 1:B:54:ASP:O     | 1:B:56:ALA:N     | 2.44                     | 0.47              |
| 1:D:125:ILE:O    | 1:D:126:ARG:C    | 2.50                     | 0.47              |
| 1:A:147:ILE:HG21 | 1:A:191:THR:HB   | 1.94                     | 0.47              |
| 1:F:184:GLU:OE1  | 1:F:184:GLU:HA   | 2.14                     | 0.47              |
| 1:E:55:PRO:HA    | 9:E:2006:HOH:O   | 2.13                     | 0.47              |
| 1:E:160:HIS:HD2  | 1:E:162:PHE:H    | 1.61                     | 0.47              |
| 1:C:122:LYS:HE2  | 1:C:139:THR:CG2  | 2.36                     | 0.47              |
| 1:E:157:PRO:HG2  | 1:E:158:HIS:CE1  | 2.49                     | 0.47              |
| 1:F:64:VAL:HG12  | 1:F:65:ASN:N     | 2.30                     | 0.47              |
| 1:B:136:TYR:CE1  | 1:B:138:GLY:HA3  | 2.50                     | 0.47              |
| 1:C:52:LYS:HB2   | 1:C:57:LEU:HD12  | 1.95                     | 0.47              |
| 1:E:198:TYR:CE2  | 4:E:1211:EPE:H32 | 2.49                     | 0.47              |
| 1:A:134:ARG:CD   | 1:A:134:ARG:H    | 2.05                     | 0.47              |
| 1:D:136:TYR:CZ   | 1:D:138:GLY:HA3  | 2.49                     | 0.47              |
| 1:D:181:ARG:HB2  | 1:D:183:GLU:CG   | 2.41                     | 0.47              |
| 1:E:202:ASP:HA   | 9:E:2027:HOH:O   | 2.14                     | 0.47              |
| 1:C:59:ILE:CG2   | 1:C:60:LYS:H     | 2.27                     | 0.46              |
| 1:C:167:TYR:O    | 1:C:170:LYS:HB2  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:129:ILE:HG22 | 1:G:136:TYR:HB2  | 1.97                     | 0.46              |
| 1:C:97:LEU:HB3   | 1:C:99:PHE:CZ    | 2.50                     | 0.46              |
| 1:A:80:LEU:C     | 1:A:82:PHE:H     | 2.19                     | 0.46              |
| 1:E:129:ILE:HG22 | 1:E:136:TYR:HB2  | 1.98                     | 0.46              |
| 1:H:49:THR:O     | 1:H:110:LYS:HA   | 2.15                     | 0.46              |
| 1:E:99:PHE:HB3   | 1:E:101:PHE:CZ   | 2.51                     | 0.46              |
| 1:E:160:HIS:CD2  | 1:E:162:PHE:HB2  | 2.51                     | 0.46              |
| 1:B:99:PHE:HB3   | 1:B:101:PHE:CZ   | 2.49                     | 0.46              |
| 1:C:101:PHE:HB2  | 1:C:105:SER:OG   | 2.16                     | 0.46              |
| 1:A:173:GLN:O    | 1:A:174:GLU:C    | 2.54                     | 0.46              |
| 1:A:181:ARG:HD3  | 1:A:183:GLU:OE2  | 2.16                     | 0.46              |
| 1:F:82:PHE:CD1   | 1:F:100:PRO:HB3  | 2.51                     | 0.46              |
| 1:G:48:THR:HG22  | 1:G:49:THR:H     | 1.80                     | 0.46              |
| 1:G:136:TYR:CZ   | 1:G:203:ILE:HD13 | 2.51                     | 0.46              |
| 1:H:125:ILE:O    | 1:H:126:ARG:C    | 2.53                     | 0.46              |
| 1:D:55:PRO:O     | 1:D:56:ALA:HB3   | 2.15                     | 0.46              |
| 1:H:48:THR:HG22  | 1:H:49:THR:N     | 2.31                     | 0.46              |
| 1:G:80:LEU:C     | 1:G:82:PHE:H     | 2.19                     | 0.46              |
| 1:D:101:PHE:CE1  | 1:D:108:VAL:HG11 | 2.51                     | 0.46              |
| 1:D:203:ILE:HA   | 1:D:204:PRO:HD2  | 1.78                     | 0.46              |
| 1:B:47:LYS:HG2   | 1:B:114:HIS:HA   | 1.97                     | 0.46              |
| 1:C:80:LEU:C     | 1:C:82:PHE:H     | 2.19                     | 0.46              |
| 1:C:99:PHE:HB3   | 1:C:101:PHE:CZ   | 2.50                     | 0.46              |
| 1:G:99:PHE:HB3   | 1:G:101:PHE:CZ   | 2.51                     | 0.46              |
| 1:D:82:PHE:CG    | 1:D:100:PRO:HB3  | 2.50                     | 0.46              |
| 1:C:181:ARG:NH2  | 1:C:183:GLU:OE1  | 2.49                     | 0.46              |
| 1:C:157:PRO:HG2  | 1:C:158:HIS:CE1  | 2.51                     | 0.46              |
| 1:B:64:VAL:O     | 1:B:94:LYS:HB3   | 2.16                     | 0.46              |
| 1:G:77:ASN:O     | 1:G:77:ASN:ND2   | 2.48                     | 0.46              |
| 1:G:108:VAL:C    | 1:G:109:LYS:HG3  | 2.36                     | 0.45              |
| 1:D:118:LEU:HD12 | 1:D:119:TYR:N    | 2.31                     | 0.45              |
| 1:F:181:ARG:O    | 1:F:183:GLU:N    | 2.50                     | 0.45              |
| 1:A:72:ASP:O     | 1:A:76:ARG:HD2   | 2.17                     | 0.45              |
| 1:A:101:PHE:HB2  | 1:A:105:SER:OG   | 2.17                     | 0.45              |
| 1:E:157:PRO:HG2  | 1:E:158:HIS:ND1  | 2.31                     | 0.45              |
| 1:E:160:HIS:HD2  | 1:E:162:PHE:HB2  | 1.82                     | 0.45              |
| 1:D:52:LYS:HG3   | 1:D:59:ILE:HD11  | 1.98                     | 0.45              |
| 1:C:59:ILE:HG22  | 1:C:60:LYS:H     | 1.82                     | 0.45              |
| 1:E:181:ARG:HD3  | 1:E:183:GLU:OE2  | 2.17                     | 0.45              |
| 1:G:181:ARG:HB2  | 1:G:183:GLU:CG   | 2.47                     | 0.45              |
| 1:D:181:ARG:O    | 1:D:182:GLY:C    | 2.54                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:162:PHE:CE2  | 1:C:188:TRP:HH2  | 2.34                     | 0.45              |
| 1:C:54:ASP:OD1   | 1:C:56:ALA:HB3   | 2.17                     | 0.45              |
| 1:E:108:VAL:HG12 | 1:E:109:LYS:N    | 2.32                     | 0.45              |
| 1:A:112:PHE:CD2  | 1:A:113:GLY:N    | 2.84                     | 0.45              |
| 1:C:130:ILE:O    | 3:C:1209:SO4:O1  | 2.35                     | 0.45              |
| 1:A:47:LYS:HA    | 1:A:116:PHE:O    | 2.16                     | 0.45              |
| 1:F:136:TYR:CE1  | 1:F:138:GLY:HA3  | 2.51                     | 0.45              |
| 1:E:80:LEU:C     | 1:E:82:PHE:H     | 2.20                     | 0.45              |
| 1:A:39:ILE:CD1   | 1:A:119:TYR:HE2  | 2.30                     | 0.45              |
| 1:H:136:TYR:CE1  | 1:H:138:GLY:HA3  | 2.52                     | 0.45              |
| 1:C:142:ILE:HG22 | 1:C:143:THR:O    | 2.17                     | 0.45              |
| 1:C:40:HIS:C     | 1:C:42:PHE:H     | 2.19                     | 0.45              |
| 1:E:73:ARG:HD3   | 1:E:98:TRP:CZ2   | 2.52                     | 0.45              |
| 1:E:87:PHE:C     | 1:E:87:PHE:CD1   | 2.91                     | 0.45              |
| 1:H:83:THR:HG21  | 1:H:124:TYR:OH   | 2.16                     | 0.45              |
| 1:D:173:GLN:O    | 1:D:174:GLU:C    | 2.55                     | 0.45              |
| 1:F:101:PHE:CE1  | 1:F:108:VAL:HG11 | 2.52                     | 0.45              |
| 1:G:157:PRO:HG2  | 1:G:158:HIS:ND1  | 2.31                     | 0.45              |
| 1:E:136:TYR:CZ   | 1:E:203:ILE:HD13 | 2.51                     | 0.45              |
| 1:F:82:PHE:CG    | 1:F:100:PRO:HB3  | 2.51                     | 0.44              |
| 1:A:48:THR:HG22  | 1:A:49:THR:H     | 1.82                     | 0.44              |
| 1:F:44:LYS:HD3   | 1:F:119:TYR:CZ   | 2.51                     | 0.44              |
| 1:C:113:GLY:HA2  | 9:C:2007:HOH:O   | 2.17                     | 0.44              |
| 1:A:157:PRO:HG2  | 1:A:158:HIS:CE1  | 2.52                     | 0.44              |
| 1:D:155:MET:HE3  | 1:D:163:LEU:HD21 | 1.99                     | 0.44              |
| 1:H:47:LYS:N     | 1:H:47:LYS:HD2   | 2.32                     | 0.44              |
| 1:H:171:ASP:OD1  | 1:H:173:GLN:HG2  | 2.17                     | 0.44              |
| 1:E:51:ILE:O     | 1:E:109:LYS:N    | 2.48                     | 0.44              |
| 1:B:170:LYS:HD2  | 5:B:1209:IDS:O3S | 2.17                     | 0.44              |
| 1:G:101:PHE:CD1  | 1:G:108:VAL:HG21 | 2.53                     | 0.44              |
| 1:G:108:VAL:HG12 | 1:G:109:LYS:N    | 2.33                     | 0.44              |
| 1:D:115:GLU:HG2  | 1:D:116:PHE:N    | 2.31                     | 0.44              |
| 1:D:48:THR:HG22  | 1:D:49:THR:N     | 2.33                     | 0.44              |
| 1:D:50:LEU:HD11  | 1:D:118:LEU:CD2  | 2.47                     | 0.44              |
| 1:A:129:ILE:HG22 | 1:A:136:TYR:HB2  | 1.98                     | 0.44              |
| 1:G:104:MET:CE   | 1:G:137:LYS:HB2  | 2.47                     | 0.44              |
| 1:F:48:THR:HG22  | 1:F:49:THR:N     | 2.33                     | 0.44              |
| 1:F:50:LEU:HD22  | 1:F:99:PHE:CE2   | 2.52                     | 0.44              |
| 1:E:165:SER:O    | 1:E:167:TYR:N    | 2.47                     | 0.44              |
| 1:E:77:ASN:O     | 1:E:77:ASN:ND2   | 2.48                     | 0.44              |
| 1:A:203:ILE:HA   | 1:A:204:PRO:HD2  | 1.87                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:101:PHE:CE1  | 1:H:108:VAL:HG11  | 2.52                     | 0.44              |
| 1:E:48:THR:O     | 1:E:116:PHE:HB3   | 2.17                     | 0.44              |
| 1:A:53:ILE:N     | 1:A:107:GLY:O     | 2.46                     | 0.44              |
| 1:H:63:LYS:HA    | 1:H:95:GLN:CB     | 2.48                     | 0.43              |
| 1:D:51:ILE:N     | 1:D:51:ILE:HD12   | 2.33                     | 0.43              |
| 1:F:93:ARG:HE    | 1:F:93:ARG:HB2    | 1.44                     | 0.43              |
| 1:B:48:THR:HG22  | 1:B:49:THR:N      | 2.33                     | 0.43              |
| 1:H:136:TYR:CZ   | 1:H:203:ILE:HD13  | 2.53                     | 0.43              |
| 1:A:181:ARG:HB2  | 1:A:183:GLU:HG3   | 1.99                     | 0.43              |
| 1:C:198:TYR:CE2  | 4:C:1219:EPE:H102 | 2.52                     | 0.43              |
| 1:G:147:ILE:CG2  | 1:G:191:THR:HB    | 2.49                     | 0.43              |
| 1:H:152:TRP:N    | 9:H:2010:HOH:O    | 2.50                     | 0.43              |
| 1:H:117:ASP:HB3  | 1:H:119:TYR:CE1   | 2.53                     | 0.43              |
| 1:A:87:PHE:CD1   | 1:A:87:PHE:C      | 2.91                     | 0.43              |
| 1:H:99:PHE:HB3   | 1:H:101:PHE:CZ    | 2.54                     | 0.43              |
| 1:B:93:ARG:HG3   | 1:B:93:ARG:NH1    | 2.32                     | 0.43              |
| 1:A:80:LEU:HA    | 1:A:81:PRO:HD2    | 1.90                     | 0.43              |
| 1:D:113:GLY:C    | 1:D:115:GLU:N     | 2.72                     | 0.43              |
| 1:A:160:HIS:HD2  | 1:A:162:PHE:N     | 2.06                     | 0.43              |
| 1:D:47:LYS:CA    | 1:D:116:PHE:O     | 2.66                     | 0.43              |
| 1:G:64:VAL:HG23  | 1:G:65:ASN:N      | 2.34                     | 0.43              |
| 1:D:180:PRO:HD2  | 9:D:2020:HOH:O    | 2.19                     | 0.43              |
| 1:A:59:ILE:CG2   | 1:A:60:LYS:H      | 2.32                     | 0.43              |
| 1:G:181:ARG:O    | 1:G:182:GLY:C     | 2.57                     | 0.43              |
| 1:A:48:THR:O     | 1:A:116:PHE:HB3   | 2.18                     | 0.43              |
| 1:E:80:LEU:HA    | 1:E:81:PRO:HD2    | 1.91                     | 0.43              |
| 1:H:85:LYS:HE2   | 1:H:124:TYR:CE2   | 2.54                     | 0.43              |
| 1:F:130:ILE:HD12 | 3:F:1216:SO4:O1   | 2.19                     | 0.42              |
| 1:D:113:GLY:O    | 1:D:115:GLU:N     | 2.52                     | 0.42              |
| 1:E:76:ARG:O     | 1:E:77:ASN:C      | 2.58                     | 0.42              |
| 1:A:118:LEU:C    | 1:A:119:TYR:HD1   | 2.22                     | 0.42              |
| 1:E:112:PHE:CG   | 1:E:113:GLY:N     | 2.87                     | 0.42              |
| 1:C:147:ILE:CG2  | 1:C:191:THR:HB    | 2.49                     | 0.42              |
| 1:B:136:TYR:CZ   | 1:B:203:ILE:HD13  | 2.54                     | 0.42              |
| 1:B:90:ASP:OD2   | 1:B:116:PHE:HE1   | 2.01                     | 0.42              |
| 1:G:203:ILE:HA   | 1:G:204:PRO:HD2   | 1.87                     | 0.42              |
| 1:B:39:ILE:HG13  | 1:B:40:HIS:ND1    | 2.35                     | 0.42              |
| 1:D:198:TYR:C    | 1:D:198:TYR:CD2   | 2.92                     | 0.42              |
| 1:F:136:TYR:CZ   | 1:F:203:ILE:HD13  | 2.54                     | 0.42              |
| 1:H:170:LYS:CE   | 1:H:170:LYS:N     | 2.82                     | 0.42              |
| 1:D:90:ASP:OD1   | 1:D:92:ALA:HB3    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:114:HIS:CA   | 9:E:2010:HOH:O   | 2.62                     | 0.42              |
| 1:E:147:ILE:CG2  | 1:E:191:THR:HB   | 2.49                     | 0.42              |
| 1:B:40:HIS:NE2   | 9:B:2001:HOH:O   | 2.37                     | 0.42              |
| 1:G:178:ARG:O    | 1:G:187:PRO:HA   | 2.20                     | 0.42              |
| 1:B:44:LYS:HE3   | 1:B:117:ASP:OD2  | 2.19                     | 0.42              |
| 1:D:90:ASP:O     | 1:D:94:LYS:N     | 2.52                     | 0.42              |
| 1:F:112:PHE:CD1  | 1:F:113:GLY:N    | 2.88                     | 0.42              |
| 1:H:90:ASP:O     | 1:H:94:LYS:HA    | 2.19                     | 0.42              |
| 1:C:136:TYR:CZ   | 1:C:203:ILE:HD13 | 2.55                     | 0.42              |
| 1:C:90:ASP:OD1   | 1:C:92:ALA:HB3   | 2.20                     | 0.42              |
| 1:C:115:GLU:N    | 1:C:115:GLU:OE1  | 2.41                     | 0.42              |
| 1:E:181:ARG:HB2  | 1:E:183:GLU:HG3  | 2.02                     | 0.42              |
| 1:F:64:VAL:CG1   | 1:F:69:GLN:HB2   | 2.46                     | 0.42              |
| 7:C:1212:SGN:O4S | 1:F:134:ARG:HG2  | 2.20                     | 0.42              |
| 1:C:161:SER:O    | 1:C:163:LEU:HG   | 2.19                     | 0.42              |
| 1:B:67:ALA:HB2   | 1:B:89:PHE:CD2   | 2.55                     | 0.42              |
| 1:B:63:LYS:HA    | 1:B:95:GLN:HB3   | 2.01                     | 0.42              |
| 1:H:170:LYS:HE3  | 1:H:170:LYS:HA   | 2.02                     | 0.42              |
| 1:E:48:THR:HG22  | 1:E:49:THR:H     | 1.85                     | 0.42              |
| 1:D:67:ALA:HB2   | 1:D:89:PHE:CD2   | 2.55                     | 0.42              |
| 1:D:57:LEU:HA    | 1:D:57:LEU:HD23  | 1.85                     | 0.42              |
| 1:D:52:LYS:CG    | 1:D:59:ILE:HD11  | 2.50                     | 0.41              |
| 1:D:122:LYS:C    | 1:D:124:TYR:H    | 2.23                     | 0.41              |
| 1:E:178:ARG:O    | 1:E:187:PRO:HA   | 2.20                     | 0.41              |
| 1:E:73:ARG:HD3   | 1:E:98:TRP:CH2   | 2.55                     | 0.41              |
| 1:A:157:PRO:HG2  | 1:A:158:HIS:ND1  | 2.35                     | 0.41              |
| 1:C:87:PHE:C     | 1:C:87:PHE:CD1   | 2.94                     | 0.41              |
| 1:E:181:ARG:NH1  | 1:E:183:GLU:OE2  | 2.53                     | 0.41              |
| 1:E:46:ALA:O     | 1:E:47:LYS:C     | 2.59                     | 0.41              |
| 1:C:181:ARG:HH21 | 1:C:183:GLU:CD   | 2.23                     | 0.41              |
| 1:F:99:PHE:HB3   | 1:F:101:PHE:CZ   | 2.55                     | 0.41              |
| 1:B:152:TRP:CD2  | 1:B:172:LEU:HD22 | 2.55                     | 0.41              |
| 1:E:102:ASN:O    | 1:E:105:SER:OG   | 2.38                     | 0.41              |
| 1:C:48:THR:HG22  | 1:C:49:THR:H     | 1.84                     | 0.41              |
| 1:C:112:PHE:CD2  | 1:C:113:GLY:N    | 2.89                     | 0.41              |
| 1:G:180:PRO:HD2  | 9:G:2014:HOH:O   | 2.20                     | 0.41              |
| 1:D:47:LYS:HA    | 1:D:116:PHE:O    | 2.21                     | 0.41              |
| 1:A:71:ALA:HA    | 1:A:87:PHE:CE2   | 2.55                     | 0.41              |
| 1:H:67:ALA:HB2   | 1:H:89:PHE:CD2   | 2.56                     | 0.41              |
| 1:G:87:PHE:CD1   | 1:G:87:PHE:C     | 2.94                     | 0.41              |
| 1:C:64:VAL:HG23  | 1:C:65:ASN:N     | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:162:PHE:HA   | 1:F:167:TYR:HE2  | 1.86                     | 0.41              |
| 1:A:132:LYS:HG3  | 1:A:134:ARG:NH2  | 2.34                     | 0.41              |
| 1:D:181:ARG:O    | 1:D:183:GLU:N    | 2.53                     | 0.41              |
| 1:E:47:LYS:CA    | 1:E:113:GLY:O    | 2.67                     | 0.41              |
| 1:G:48:THR:CG2   | 1:G:49:THR:N     | 2.84                     | 0.41              |
| 1:A:41:GLU:HG2   | 1:B:41:GLU:CG    | 2.49                     | 0.41              |
| 1:E:133:GLY:O    | 1:E:134:ARG:C    | 2.56                     | 0.41              |
| 1:G:174:GLU:HB2  | 1:G:176:TYR:CE2  | 2.56                     | 0.41              |
| 1:B:61:THR:HA    | 1:B:96:CYS:O     | 2.21                     | 0.41              |
| 1:C:157:PRO:HG2  | 1:C:158:HIS:ND1  | 2.36                     | 0.41              |
| 1:C:197:ARG:HD3  | 9:C:2027:HOH:O   | 2.21                     | 0.41              |
| 1:F:198:TYR:C    | 1:F:198:TYR:CD1  | 2.95                     | 0.41              |
| 1:F:44:LYS:HA    | 1:F:118:LEU:O    | 2.21                     | 0.41              |
| 1:D:152:TRP:CD2  | 1:D:172:LEU:HD22 | 2.56                     | 0.41              |
| 1:C:48:THR:CG2   | 1:C:49:THR:N     | 2.85                     | 0.40              |
| 1:H:44:LYS:HA    | 1:H:118:LEU:O    | 2.21                     | 0.40              |
| 6:B:1223:IDS:O61 | 6:B:1224:SGN:H3  | 2.21                     | 0.40              |
| 1:B:64:VAL:HG13  | 1:B:65:ASN:H     | 1.86                     | 0.40              |
| 1:D:133:GLY:N    | 9:D:2008:HOH:O   | 2.35                     | 0.40              |
| 1:A:77:ASN:CB    | 1:B:142:ILE:HG12 | 2.51                     | 0.40              |
| 1:F:135:SER:OG   | 3:F:1216:SO4:S   | 2.78                     | 0.40              |
| 1:A:178:ARG:O    | 1:A:187:PRO:HA   | 2.21                     | 0.40              |
| 1:D:141:SER:C    | 1:D:142:ILE:HD12 | 2.41                     | 0.40              |
| 1:A:108:VAL:C    | 1:A:109:LYS:HG3  | 2.42                     | 0.40              |
| 1:A:136:TYR:CZ   | 1:A:203:ILE:HD13 | 2.57                     | 0.40              |
| 1:F:100:PRO:HD2  | 1:F:101:PHE:CE2  | 2.57                     | 0.40              |
| 1:F:152:TRP:CD2  | 1:F:172:LEU:HD22 | 2.57                     | 0.40              |
| 1:B:164:PRO:O    | 1:B:168:ARG:N    | 2.55                     | 0.40              |
| 1:E:90:ASP:O     | 1:E:92:ALA:N     | 2.54                     | 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     | 170/183 (93%)   | 152 (89%)  | 15 (9%)   | 3 (2%)   | 11          | 45 |
| 1   | B     | 170/183 (93%)   | 152 (89%)  | 17 (10%)  | 1 (1%)   | 30          | 72 |
| 1   | C     | 170/183 (93%)   | 147 (86%)  | 22 (13%)  | 1 (1%)   | 30          | 72 |
| 1   | D     | 170/183 (93%)   | 148 (87%)  | 18 (11%)  | 4 (2%)   | 7           | 35 |
| 1   | E     | 171/183 (93%)   | 148 (86%)  | 18 (10%)  | 5 (3%)   | 6           | 29 |
| 1   | F     | 171/183 (93%)   | 149 (87%)  | 18 (10%)  | 4 (2%)   | 8           | 36 |
| 1   | G     | 160/183 (87%)   | 142 (89%)  | 14 (9%)   | 4 (2%)   | 7           | 34 |
| 1   | H     | 169/183 (92%)   | 147 (87%)  | 21 (12%)  | 1 (1%)   | 30          | 72 |
| All | All   | 1351/1464 (92%) | 1185 (88%) | 143 (11%) | 23 (2%)  | 11          | 46 |

All (23) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 38  | THR  |
| 1   | E     | 77  | ASN  |
| 1   | E     | 91  | LYS  |
| 1   | F     | 55  | PRO  |
| 1   | F     | 182 | GLY  |
| 1   | H     | 94  | LYS  |
| 1   | A     | 94  | LYS  |
| 1   | D     | 55  | PRO  |
| 1   | E     | 167 | TYR  |
| 1   | C     | 162 | PHE  |
| 1   | D     | 114 | HIS  |
| 1   | F     | 54  | ASP  |
| 1   | B     | 54  | ASP  |
| 1   | E     | 166 | SER  |
| 1   | G     | 77  | ASN  |
| 1   | G     | 91  | LYS  |
| 1   | D     | 53  | ILE  |
| 1   | D     | 59  | ILE  |
| 1   | F     | 100 | PRO  |
| 1   | G     | 182 | GLY  |
| 1   | A     | 81  | PRO  |
| 1   | E     | 81  | PRO  |
| 1   | G     | 81  | 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     | 140/165 (85%)   | 133 (95%)  | 7 (5%)   | 30          | 70 |
| 1   | B     | 144/165 (87%)   | 140 (97%)  | 4 (3%)   | 51          | 84 |
| 1   | C     | 145/165 (88%)   | 141 (97%)  | 4 (3%)   | 51          | 84 |
| 1   | D     | 137/165 (83%)   | 130 (95%)  | 7 (5%)   | 29          | 69 |
| 1   | E     | 132/165 (80%)   | 129 (98%)  | 3 (2%)   | 58          | 87 |
| 1   | F     | 141/165 (86%)   | 135 (96%)  | 6 (4%)   | 35          | 75 |
| 1   | G     | 129/165 (78%)   | 125 (97%)  | 4 (3%)   | 47          | 83 |
| 1   | H     | 135/165 (82%)   | 128 (95%)  | 7 (5%)   | 29          | 68 |
| All | All   | 1103/1320 (84%) | 1061 (96%) | 42 (4%)  | 40          | 78 |

All (42) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 76  | ARG  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 104 | MET  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 165 | SER  |
| 1   | A     | 191 | THR  |
| 1   | A     | 208 | GLU  |
| 1   | B     | 73  | ARG  |
| 1   | B     | 77  | ASN  |
| 1   | B     | 170 | LYS  |
| 1   | B     | 191 | THR  |
| 1   | C     | 77  | ASN  |
| 1   | C     | 142 | ILE  |
| 1   | C     | 191 | THR  |
| 1   | C     | 195 | GLU  |
| 1   | D     | 52  | LYS  |
| 1   | D     | 77  | ASN  |
| 1   | D     | 115 | GLU  |
| 1   | D     | 117 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 134 | ARG  |
| 1   | D     | 165 | SER  |
| 1   | D     | 191 | THR  |
| 1   | E     | 76  | ARG  |
| 1   | E     | 77  | ASN  |
| 1   | E     | 191 | THR  |
| 1   | F     | 73  | ARG  |
| 1   | F     | 77  | ASN  |
| 1   | F     | 134 | ARG  |
| 1   | F     | 191 | THR  |
| 1   | F     | 198 | TYR  |
| 1   | F     | 209 | VAL  |
| 1   | G     | 77  | ASN  |
| 1   | G     | 132 | LYS  |
| 1   | G     | 159 | GLU  |
| 1   | G     | 191 | THR  |
| 1   | H     | 77  | ASN  |
| 1   | H     | 117 | ASP  |
| 1   | H     | 123 | ASP  |
| 1   | H     | 134 | ARG  |
| 1   | H     | 170 | LYS  |
| 1   | H     | 191 | THR  |
| 1   | H     | 202 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 65  | ASN  |
| 1   | A     | 160 | HIS  |
| 1   | B     | 65  | ASN  |
| 1   | B     | 158 | HIS  |
| 1   | C     | 160 | HIS  |
| 1   | C     | 173 | GLN  |
| 1   | D     | 65  | ASN  |
| 1   | D     | 158 | HIS  |
| 1   | E     | 160 | HIS  |
| 1   | F     | 40  | HIS  |
| 1   | F     | 65  | ASN  |
| 1   | F     | 158 | HIS  |
| 1   | G     | 65  | ASN  |
| 1   | G     | 160 | HIS  |
| 1   | G     | 205 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 158 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

42 carbohydrates are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | IDS  | A     | 1209 | 2    | 13,17,17     | 0.81 | 0           | 19,26,26    | 1.62 | 4 (21%)     |
| 2   | SGN  | A     | 1210 | 2    | 17,19,20     | 1.17 | 2 (11%)     | 19,29,31    | 1.98 | 3 (15%)     |
| 2   | IDS  | A     | 1211 | 2    | 13,16,17     | 1.41 | 1 (7%)      | 17,24,26    | 2.97 | 4 (23%)     |
| 2   | SGN  | A     | 1212 | 2    | 17,19,20     | 1.27 | 3 (17%)     | 19,29,31    | 1.93 | 4 (21%)     |
| 2   | IDS  | A     | 1213 | 2    | 13,16,17     | 1.31 | 2 (15%)     | 17,24,26    | 3.67 | 2 (11%)     |
| 2   | SGN  | A     | 1214 | 2    | 16,18,20     | 1.41 | 1 (6%)      | 15,27,31    | 1.31 | 2 (13%)     |
| 5   | IDS  | B     | 1209 | 5    | 13,17,17     | 1.06 | 0           | 19,26,26    | 2.66 | 4 (21%)     |
| 5   | SGN  | B     | 1210 | 5    | 17,19,20     | 1.12 | 1 (5%)      | 19,29,31    | 1.67 | 3 (15%)     |
| 5   | IDS  | B     | 1211 | 5    | 13,16,17     | 1.46 | 2 (15%)     | 17,24,26    | 2.07 | 5 (29%)     |
| 5   | SGN  | B     | 1212 | 5    | 17,19,20     | 1.00 | 0           | 19,29,31    | 1.92 | 4 (21%)     |
| 5   | IDS  | B     | 1213 | 5    | 13,16,17     | 1.47 | 2 (15%)     | 17,24,26    | 1.80 | 4 (23%)     |
| 5   | SGN  | B     | 1214 | 5    | 17,19,20     | 1.24 | 2 (11%)     | 19,29,31    | 1.80 | 4 (21%)     |
| 5   | IDS  | B     | 1215 | 5    | 12,15,17     | 1.58 | 4 (33%)     | 12,22,26    | 0.87 | 0           |
| 6   | IDS  | B     | 1217 | 6    | 13,17,17     | 1.27 | 1 (7%)      | 19,26,26    | 2.54 | 4 (21%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | SGN  | B     | 1218 | 6    | 17,19,20     | 1.24 | 1 (5%)   | 19,29,31    | 1.56 | 4 (21%)  |
| 6   | IDS  | B     | 1219 | 6    | 13,16,17     | 1.38 | 2 (15%)  | 17,24,26    | 1.30 | 2 (11%)  |
| 6   | SGN  | B     | 1220 | 6    | 17,19,20     | 0.94 | 0        | 19,29,31    | 1.59 | 4 (21%)  |
| 6   | IDS  | B     | 1221 | 6    | 13,16,17     | 1.41 | 2 (15%)  | 17,24,26    | 2.86 | 4 (23%)  |
| 6   | SGN  | B     | 1222 | 6    | 17,19,20     | 1.32 | 3 (17%)  | 19,29,31    | 2.13 | 3 (15%)  |
| 6   | IDS  | B     | 1223 | 6    | 13,16,17     | 1.46 | 2 (15%)  | 17,24,26    | 3.77 | 3 (17%)  |
| 6   | SGN  | B     | 1224 | 6    | 16,18,20     | 1.45 | 3 (18%)  | 15,27,31    | 1.22 | 2 (13%)  |
| 7   | SGN  | C     | 1210 | 7    | 18,20,20     | 1.36 | 3 (16%)  | 20,31,31    | 2.64 | 6 (30%)  |
| 7   | IDS  | C     | 1211 | 7    | 13,16,17     | 1.56 | 4 (30%)  | 17,24,26    | 2.25 | 3 (17%)  |
| 7   | SGN  | C     | 1212 | 7    | 17,19,20     | 1.07 | 1 (5%)   | 19,29,31    | 1.92 | 5 (26%)  |
| 7   | IDS  | C     | 1213 | 7    | 13,16,17     | 1.21 | 2 (15%)  | 17,24,26    | 1.79 | 3 (17%)  |
| 7   | SGN  | C     | 1214 | 7    | 17,19,20     | 0.86 | 0        | 19,29,31    | 1.45 | 4 (21%)  |
| 7   | IDS  | C     | 1215 | 7    | 13,16,17     | 1.37 | 2 (15%)  | 17,24,26    | 1.37 | 3 (17%)  |
| 7   | SGN  | C     | 1216 | 7    | 17,19,20     | 1.10 | 1 (5%)   | 19,29,31    | 2.20 | 5 (26%)  |
| 7   | IDS  | C     | 1217 | 7    | 13,16,17     | 1.39 | 2 (15%)  | 17,24,26    | 1.09 | 1 (5%)   |
| 7   | SGN  | C     | 1218 | 7    | 16,18,20     | 1.28 | 3 (18%)  | 15,27,31    | 1.40 | 2 (13%)  |
| 8   | SGN  | F     | 1210 | 8    | 18,20,20     | 1.28 | 3 (16%)  | 20,31,31    | 1.32 | 1 (5%)   |
| 8   | IDS  | F     | 1211 | 8    | 13,16,17     | 1.41 | 2 (15%)  | 17,24,26    | 1.75 | 4 (23%)  |
| 8   | SGN  | F     | 1212 | 8    | 17,19,20     | 1.14 | 2 (11%)  | 19,29,31    | 1.95 | 4 (21%)  |
| 8   | IDS  | F     | 1213 | 8    | 13,16,17     | 1.40 | 2 (15%)  | 17,24,26    | 2.31 | 4 (23%)  |
| 8   | SGN  | F     | 1214 | 8    | 17,19,20     | 1.17 | 1 (5%)   | 19,29,31    | 2.02 | 3 (15%)  |
| 8   | IDS  | F     | 1215 | 8    | 12,15,17     | 1.53 | 2 (16%)  | 12,22,26    | 0.90 | 0        |
| 8   | SGN  | G     | 1209 | 8    | 18,20,20     | 1.29 | 2 (11%)  | 20,31,31    | 2.72 | 2 (10%)  |
| 8   | IDS  | G     | 1210 | 8    | 13,16,17     | 1.42 | 1 (7%)   | 17,24,26    | 1.74 | 2 (11%)  |
| 8   | SGN  | G     | 1211 | 8    | 17,19,20     | 1.23 | 2 (11%)  | 19,29,31    | 2.23 | 4 (21%)  |
| 8   | IDS  | G     | 1212 | 8    | 13,16,17     | 1.47 | 2 (15%)  | 17,24,26    | 2.95 | 5 (29%)  |
| 8   | SGN  | G     | 1213 | 8    | 17,19,20     | 1.39 | 3 (17%)  | 19,29,31    | 1.86 | 3 (15%)  |
| 8   | IDS  | G     | 1214 | 8    | 12,15,17     | 1.47 | 2 (16%)  | 12,22,26    | 0.97 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | IDS  | A     | 1209 | 2    | -       | 0/5/29/29 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | SGN  | A     | 1210 | 2    | -       | 0/11/28/31 | 0/1/1/1 |
| 2   | IDS  | A     | 1211 | 2    | -       | 0/5/26/29  | 0/1/1/1 |
| 2   | SGN  | A     | 1212 | 2    | -       | 0/11/28/31 | 0/1/1/1 |
| 2   | IDS  | A     | 1213 | 2    | 1/1/6/7 | 0/5/26/29  | 0/1/1/1 |
| 2   | SGN  | A     | 1214 | 2    | -       | 0/11/24/31 | 0/1/1/1 |
| 5   | IDS  | B     | 1209 | 5    | -       | 0/5/29/29  | 0/1/1/1 |
| 5   | SGN  | B     | 1210 | 5    | -       | 0/11/28/31 | 0/1/1/1 |
| 5   | IDS  | B     | 1211 | 5    | -       | 0/5/26/29  | 0/1/1/1 |
| 5   | SGN  | B     | 1212 | 5    | -       | 0/11/28/31 | 0/1/1/1 |
| 5   | IDS  | B     | 1213 | 5    | -       | 0/5/26/29  | 0/1/1/1 |
| 5   | SGN  | B     | 1214 | 5    | -       | 0/11/28/31 | 0/1/1/1 |
| 5   | IDS  | B     | 1215 | 5    | -       | 0/5/22/29  | 1/1/1/1 |
| 6   | IDS  | B     | 1217 | 6    | -       | 1/5/29/29  | 0/1/1/1 |
| 6   | SGN  | B     | 1218 | 6    | -       | 0/11/28/31 | 0/1/1/1 |
| 6   | IDS  | B     | 1219 | 6    | -       | 0/5/26/29  | 0/1/1/1 |
| 6   | SGN  | B     | 1220 | 6    | -       | 0/11/28/31 | 0/1/1/1 |
| 6   | IDS  | B     | 1221 | 6    | -       | 0/5/26/29  | 0/1/1/1 |
| 6   | SGN  | B     | 1222 | 6    | -       | 0/11/28/31 | 0/1/1/1 |
| 6   | IDS  | B     | 1223 | 6    | 1/1/6/7 | 0/5/26/29  | 0/1/1/1 |
| 6   | SGN  | B     | 1224 | 6    | -       | 0/11/24/31 | 0/1/1/1 |
| 7   | SGN  | C     | 1210 | 7    | -       | 0/11/31/31 | 0/1/1/1 |
| 7   | IDS  | C     | 1211 | 7    | -       | 0/5/26/29  | 0/1/1/1 |
| 7   | SGN  | C     | 1212 | 7    | -       | 0/11/28/31 | 0/1/1/1 |
| 7   | IDS  | C     | 1213 | 7    | -       | 0/5/26/29  | 0/1/1/1 |
| 7   | SGN  | C     | 1214 | 7    | -       | 0/11/28/31 | 0/1/1/1 |
| 7   | IDS  | C     | 1215 | 7    | -       | 0/5/26/29  | 0/1/1/1 |
| 7   | SGN  | C     | 1216 | 7    | -       | 0/11/28/31 | 0/1/1/1 |
| 7   | IDS  | C     | 1217 | 7    | -       | 0/5/26/29  | 0/1/1/1 |
| 7   | SGN  | C     | 1218 | 7    | -       | 0/11/24/31 | 0/1/1/1 |
| 8   | SGN  | F     | 1210 | 8    | -       | 0/11/31/31 | 0/1/1/1 |
| 8   | IDS  | F     | 1211 | 8    | -       | 0/5/26/29  | 0/1/1/1 |
| 8   | SGN  | F     | 1212 | 8    | -       | 0/11/28/31 | 0/1/1/1 |
| 8   | IDS  | F     | 1213 | 8    | -       | 0/5/26/29  | 0/1/1/1 |
| 8   | SGN  | F     | 1214 | 8    | -       | 0/11/28/31 | 0/1/1/1 |
| 8   | IDS  | F     | 1215 | 8    | -       | 0/5/22/29  | 0/1/1/1 |
| 8   | SGN  | G     | 1209 | 8    | -       | 0/11/31/31 | 0/1/1/1 |
| 8   | IDS  | G     | 1210 | 8    | -       | 0/5/26/29  | 0/1/1/1 |
| 8   | SGN  | G     | 1211 | 8    | -       | 0/11/28/31 | 0/1/1/1 |
| 8   | IDS  | G     | 1212 | 8    | -       | 0/5/26/29  | 0/1/1/1 |
| 8   | SGN  | G     | 1213 | 8    | -       | 0/11/28/31 | 0/1/1/1 |
| 8   | IDS  | G     | 1214 | 8    | -       | 0/5/22/29  | 1/1/1/1 |

All (76) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8   | G     | 1210 | IDS  | O2-C2  | -3.79 | 1.41        | 1.47     |
| 6   | B     | 1221 | IDS  | O2-C2  | -3.76 | 1.41        | 1.47     |
| 2   | A     | 1211 | IDS  | O2-C2  | -3.67 | 1.41        | 1.47     |
| 8   | G     | 1212 | IDS  | O2-C2  | -3.59 | 1.41        | 1.47     |
| 8   | F     | 1213 | IDS  | O2-C2  | -3.53 | 1.42        | 1.47     |
| 6   | B     | 1219 | IDS  | O2-C2  | -3.53 | 1.42        | 1.47     |
| 7   | C     | 1215 | IDS  | O2-C2  | -3.52 | 1.42        | 1.47     |
| 5   | B     | 1213 | IDS  | O2-C2  | -3.08 | 1.42        | 1.47     |
| 5   | B     | 1215 | IDS  | O2-C2  | -3.04 | 1.42        | 1.47     |
| 7   | C     | 1211 | IDS  | O2-C2  | -2.97 | 1.42        | 1.47     |
| 7   | C     | 1217 | IDS  | O2-C2  | -2.72 | 1.43        | 1.47     |
| 8   | F     | 1211 | IDS  | O2-C2  | -2.70 | 1.43        | 1.47     |
| 7   | C     | 1213 | IDS  | O2-C2  | -2.56 | 1.43        | 1.47     |
| 5   | B     | 1211 | IDS  | O2-C2  | -2.48 | 1.43        | 1.47     |
| 7   | C     | 1212 | SGN  | C1-C2  | 2.00  | 1.55        | 1.52     |
| 2   | A     | 1210 | SGN  | O1S-S1 | 2.01  | 1.44        | 1.42     |
| 6   | B     | 1222 | SGN  | C4-C5  | 2.01  | 1.57        | 1.53     |
| 8   | F     | 1212 | SGN  | O2S-S1 | 2.01  | 1.44        | 1.42     |
| 5   | B     | 1214 | SGN  | C4-C5  | 2.02  | 1.57        | 1.53     |
| 8   | F     | 1210 | SGN  | O1S-S1 | 2.02  | 1.44        | 1.42     |
| 6   | B     | 1224 | SGN  | O1S-S1 | 2.03  | 1.44        | 1.42     |
| 5   | B     | 1215 | IDS  | C4-C3  | 2.08  | 1.56        | 1.52     |
| 7   | C     | 1218 | SGN  | O2S-S1 | 2.10  | 1.44        | 1.42     |
| 7   | C     | 1211 | IDS  | O5-C5  | 2.13  | 1.45        | 1.43     |
| 7   | C     | 1216 | SGN  | C1-C2  | 2.15  | 1.55        | 1.52     |
| 7   | C     | 1218 | SGN  | C1-C2  | 2.15  | 1.55        | 1.52     |
| 8   | G     | 1211 | SGN  | O2S-S1 | 2.16  | 1.44        | 1.42     |
| 6   | B     | 1224 | SGN  | C3-C2  | 2.19  | 1.55        | 1.52     |
| 6   | B     | 1221 | IDS  | C1-C2  | 2.19  | 1.55        | 1.51     |
| 2   | A     | 1213 | IDS  | C4-C5  | 2.21  | 1.58        | 1.53     |
| 5   | B     | 1210 | SGN  | C1-C2  | 2.21  | 1.55        | 1.52     |
| 2   | A     | 1212 | SGN  | O2S-S1 | 2.22  | 1.44        | 1.42     |
| 8   | G     | 1213 | SGN  | C4-C5  | 2.26  | 1.57        | 1.53     |
| 2   | A     | 1212 | SGN  | O1S-S1 | 2.27  | 1.44        | 1.42     |
| 8   | G     | 1213 | SGN  | O2S-S1 | 2.29  | 1.44        | 1.42     |
| 7   | C     | 1210 | SGN  | C1-C2  | 2.33  | 1.55        | 1.53     |
| 8   | G     | 1214 | IDS  | C4-C5  | 2.38  | 1.56        | 1.52     |
| 7   | C     | 1211 | IDS  | C4-C5  | 2.39  | 1.58        | 1.53     |
| 8   | G     | 1212 | IDS  | C1-C2  | 2.40  | 1.55        | 1.51     |
| 2   | A     | 1210 | SGN  | O2S-S1 | 2.40  | 1.44        | 1.42     |
| 8   | F     | 1214 | SGN  | C1-C2  | 2.41  | 1.55        | 1.52     |
| 7   | C     | 1215 | IDS  | C1-C2  | 2.42  | 1.55        | 1.51     |
| 5   | B     | 1215 | IDS  | C1-C2  | 2.42  | 1.55        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 8   | G     | 1209 | SGN  | O2S-S1 | 2.44 | 1.44        | 1.42     |
| 8   | F     | 1210 | SGN  | O2S-S1 | 2.47 | 1.44        | 1.42     |
| 2   | A     | 1213 | IDS  | C1-C2  | 2.49 | 1.55        | 1.51     |
| 6   | B     | 1219 | IDS  | C1-C2  | 2.52 | 1.55        | 1.51     |
| 7   | C     | 1218 | SGN  | O1S-S1 | 2.52 | 1.44        | 1.42     |
| 8   | F     | 1215 | IDS  | C4-C5  | 2.53 | 1.56        | 1.52     |
| 8   | F     | 1212 | SGN  | C1-C2  | 2.54 | 1.56        | 1.52     |
| 5   | B     | 1215 | IDS  | C4-C5  | 2.56 | 1.56        | 1.52     |
| 6   | B     | 1222 | SGN  | O2S-S1 | 2.60 | 1.44        | 1.42     |
| 6   | B     | 1217 | IDS  | C4-C5  | 2.61 | 1.59        | 1.53     |
| 6   | B     | 1223 | IDS  | C1-C2  | 2.64 | 1.56        | 1.51     |
| 8   | F     | 1213 | IDS  | C1-C2  | 2.65 | 1.56        | 1.51     |
| 7   | C     | 1213 | IDS  | C1-C2  | 2.65 | 1.56        | 1.51     |
| 8   | G     | 1209 | SGN  | C1-C2  | 2.66 | 1.56        | 1.53     |
| 7   | C     | 1210 | SGN  | O2S-S1 | 2.68 | 1.44        | 1.42     |
| 8   | G     | 1213 | SGN  | C1-C2  | 2.74 | 1.56        | 1.52     |
| 6   | B     | 1223 | IDS  | C4-C5  | 2.75 | 1.59        | 1.53     |
| 7   | C     | 1211 | IDS  | C1-C2  | 2.78 | 1.56        | 1.51     |
| 6   | B     | 1218 | SGN  | C1-C2  | 2.78 | 1.56        | 1.52     |
| 6   | B     | 1222 | SGN  | C1-C2  | 2.81 | 1.56        | 1.52     |
| 2   | A     | 1212 | SGN  | C1-C2  | 2.82 | 1.56        | 1.52     |
| 8   | F     | 1215 | IDS  | C1-C2  | 2.83 | 1.56        | 1.51     |
| 7   | C     | 1210 | SGN  | O1S-S1 | 2.85 | 1.45        | 1.42     |
| 8   | F     | 1210 | SGN  | C1-C2  | 2.86 | 1.56        | 1.53     |
| 8   | G     | 1211 | SGN  | C1-C2  | 2.88 | 1.56        | 1.52     |
| 7   | C     | 1217 | IDS  | C1-C2  | 2.89 | 1.56        | 1.51     |
| 5   | B     | 1214 | SGN  | C1-C2  | 2.94 | 1.56        | 1.52     |
| 5   | B     | 1213 | IDS  | C1-C2  | 3.07 | 1.56        | 1.51     |
| 8   | G     | 1214 | IDS  | C1-C2  | 3.22 | 1.57        | 1.51     |
| 8   | F     | 1211 | IDS  | C1-C2  | 3.26 | 1.57        | 1.51     |
| 5   | B     | 1211 | IDS  | C1-C2  | 3.50 | 1.57        | 1.51     |
| 6   | B     | 1224 | SGN  | C1-C2  | 3.56 | 1.57        | 1.52     |
| 2   | A     | 1214 | SGN  | C1-C2  | 3.77 | 1.57        | 1.52     |

All (133) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 8   | G     | 1209 | SGN  | O4-C4-C3 | -11.37 | 84.74       | 110.34   |
| 7   | C     | 1210 | SGN  | O4-C4-C3 | -10.24 | 87.27       | 110.34   |
| 8   | G     | 1212 | IDS  | O4-C4-C3 | -6.13  | 96.53       | 110.34   |
| 2   | A     | 1211 | IDS  | O4-C4-C3 | -6.09  | 96.62       | 110.34   |
| 5   | B     | 1212 | SGN  | O4-C4-C3 | -5.89  | 97.07       | 110.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | A     | 1212 | SGN  | O4-C4-C3 | -5.89 | 97.09       | 110.34   |
| 6   | B     | 1222 | SGN  | O4-C4-C3 | -5.86 | 97.14       | 110.34   |
| 6   | B     | 1221 | IDS  | O4-C4-C3 | -5.83 | 97.22       | 110.34   |
| 8   | F     | 1214 | SGN  | O4-C4-C3 | -5.62 | 97.68       | 110.34   |
| 5   | B     | 1210 | SGN  | O4-C4-C3 | -4.88 | 99.36       | 110.34   |
| 7   | C     | 1216 | SGN  | O4-C4-C3 | -4.83 | 99.46       | 110.34   |
| 8   | G     | 1211 | SGN  | O4-C4-C3 | -4.69 | 99.78       | 110.34   |
| 5   | B     | 1213 | IDS  | O4-C4-C3 | -4.48 | 100.26      | 110.34   |
| 8   | F     | 1210 | SGN  | O4-C4-C3 | -4.17 | 100.95      | 110.34   |
| 8   | F     | 1212 | SGN  | O4-C4-C3 | -4.16 | 100.96      | 110.34   |
| 8   | F     | 1213 | IDS  | O4-C4-C3 | -3.85 | 101.66      | 110.34   |
| 5   | B     | 1214 | SGN  | O4-C4-C3 | -3.64 | 102.15      | 110.34   |
| 2   | A     | 1210 | SGN  | O4-C4-C3 | -3.63 | 102.16      | 110.34   |
| 7   | C     | 1212 | SGN  | O4-C4-C3 | -3.20 | 103.14      | 110.34   |
| 6   | B     | 1220 | SGN  | O4-C4-C3 | -3.14 | 103.26      | 110.34   |
| 8   | G     | 1213 | SGN  | O4-C4-C3 | -3.14 | 103.28      | 110.34   |
| 8   | F     | 1211 | IDS  | O4-C4-C3 | -3.11 | 103.33      | 110.34   |
| 6   | B     | 1224 | SGN  | O1S-S1-N | -3.09 | 104.37      | 108.50   |
| 6   | B     | 1218 | SGN  | O4-C4-C3 | -3.03 | 103.50      | 110.34   |
| 6   | B     | 1220 | SGN  | O2S-S1-N | -3.02 | 104.46      | 108.50   |
| 7   | C     | 1214 | SGN  | O4-C4-C3 | -2.96 | 103.67      | 110.34   |
| 7   | C     | 1216 | SGN  | O2S-S1-N | -2.89 | 104.64      | 108.50   |
| 7   | C     | 1218 | SGN  | C4-C3-C2 | -2.86 | 107.38      | 111.34   |
| 7   | C     | 1215 | IDS  | O4-C4-C3 | -2.86 | 103.90      | 110.34   |
| 7   | C     | 1212 | SGN  | C4-C3-C2 | -2.84 | 106.81      | 111.23   |
| 2   | A     | 1214 | SGN  | O1S-S1-N | -2.83 | 104.72      | 108.50   |
| 7   | C     | 1217 | IDS  | O4-C4-C3 | -2.80 | 104.03      | 110.34   |
| 7   | C     | 1218 | SGN  | O1S-S1-N | -2.78 | 104.78      | 108.50   |
| 2   | A     | 1214 | SGN  | C4-C3-C2 | -2.66 | 107.66      | 111.34   |
| 7   | C     | 1210 | SGN  | O4-C4-C5 | -2.53 | 102.53      | 109.24   |
| 6   | B     | 1218 | SGN  | C4-C3-C2 | -2.51 | 107.33      | 111.23   |
| 7   | C     | 1214 | SGN  | C4-C3-C2 | -2.49 | 107.36      | 111.23   |
| 7   | C     | 1212 | SGN  | C2-N-S1  | -2.46 | 116.37      | 121.35   |
| 5   | B     | 1212 | SGN  | C4-C3-C2 | -2.32 | 107.62      | 111.23   |
| 5   | B     | 1211 | IDS  | O4-C4-C5 | -2.30 | 106.09      | 110.42   |
| 5   | B     | 1214 | SGN  | O2S-S1-N | -2.26 | 105.48      | 108.50   |
| 6   | B     | 1218 | SGN  | C2-N-S1  | -2.26 | 116.78      | 121.35   |
| 6   | B     | 1224 | SGN  | C4-C3-C2 | -2.25 | 108.23      | 111.34   |
| 8   | G     | 1211 | SGN  | C4-C3-C2 | -2.24 | 107.74      | 111.23   |
| 7   | C     | 1210 | SGN  | O2S-S1-N | -2.24 | 105.50      | 108.50   |
| 7   | C     | 1216 | SGN  | C3-C4-C5 | -2.24 | 106.30      | 110.20   |
| 2   | A     | 1212 | SGN  | C4-C3-C2 | -2.22 | 107.77      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 5   | B     | 1210 | SGN  | O2S-S1-N | -2.16 | 105.62      | 108.50   |
| 8   | F     | 1212 | SGN  | C4-C3-C2 | -2.12 | 107.93      | 111.23   |
| 8   | G     | 1209 | SGN  | C3-C4-C5 | -2.10 | 106.54      | 110.20   |
| 7   | C     | 1214 | SGN  | O2S-S1-N | -2.03 | 105.78      | 108.50   |
| 7   | C     | 1210 | SGN  | C1-O5-C5 | 2.00  | 117.18      | 113.47   |
| 6   | B     | 1223 | IDS  | C6-C5-C4 | 2.04  | 118.76      | 113.00   |
| 7   | C     | 1210 | SGN  | C6-C5-C4 | 2.09  | 116.76      | 112.03   |
| 2   | A     | 1209 | IDS  | O4-C4-C5 | 2.17  | 114.50      | 110.42   |
| 6   | B     | 1220 | SGN  | O4-C4-C5 | 2.18  | 115.01      | 109.24   |
| 8   | G     | 1212 | IDS  | C4-C3-C2 | 2.32  | 114.24      | 110.20   |
| 7   | C     | 1213 | IDS  | C1-O5-C5 | 2.34  | 115.45      | 111.84   |
| 6   | B     | 1223 | IDS  | C1-O5-C5 | 2.39  | 115.53      | 111.84   |
| 2   | A     | 1210 | SGN  | C1-O5-C5 | 2.44  | 115.35      | 112.25   |
| 2   | A     | 1209 | IDS  | C1-C2-C3 | 2.46  | 114.79      | 110.45   |
| 7   | C     | 1210 | SGN  | O6-C6-C5 | 2.49  | 112.70      | 107.90   |
| 7   | C     | 1215 | IDS  | C1-O5-C5 | 2.52  | 115.72      | 111.84   |
| 2   | A     | 1213 | IDS  | C1-O5-C5 | 2.52  | 115.72      | 111.84   |
| 5   | B     | 1213 | IDS  | O4-C4-C5 | 2.57  | 115.26      | 110.42   |
| 6   | B     | 1217 | IDS  | O2-C2-C1 | 2.60  | 111.19      | 107.65   |
| 5   | B     | 1211 | IDS  | C4-C3-C2 | 2.60  | 114.73      | 110.20   |
| 5   | B     | 1209 | IDS  | C1-O5-C5 | 2.64  | 116.11      | 112.22   |
| 8   | F     | 1211 | IDS  | C1-O5-C5 | 2.73  | 116.04      | 111.84   |
| 2   | A     | 1212 | SGN  | C1-O5-C5 | 2.74  | 115.73      | 112.25   |
| 2   | A     | 1209 | IDS  | C1-O5-C5 | 2.75  | 116.26      | 112.22   |
| 5   | B     | 1214 | SGN  | C1-O5-C5 | 2.76  | 115.75      | 112.25   |
| 8   | G     | 1212 | IDS  | C1-O5-C5 | 2.82  | 116.19      | 111.84   |
| 5   | B     | 1212 | SGN  | O4-C4-C5 | 2.83  | 116.74      | 109.24   |
| 6   | B     | 1221 | IDS  | C1-O5-C5 | 2.85  | 116.23      | 111.84   |
| 6   | B     | 1217 | IDS  | C1-O5-C5 | 2.86  | 116.43      | 112.22   |
| 2   | A     | 1211 | IDS  | C1-O5-C5 | 2.87  | 116.27      | 111.84   |
| 8   | G     | 1211 | SGN  | C1-O5-C5 | 2.88  | 115.90      | 112.25   |
| 7   | C     | 1214 | SGN  | C1-O5-C5 | 2.91  | 115.94      | 112.25   |
| 8   | F     | 1212 | SGN  | C1-O5-C5 | 2.98  | 116.03      | 112.25   |
| 5   | B     | 1211 | IDS  | C1-O5-C5 | 2.98  | 116.43      | 111.84   |
| 8   | F     | 1213 | IDS  | C1-O5-C5 | 3.00  | 116.46      | 111.84   |
| 7   | C     | 1215 | IDS  | C1-C2-C3 | 3.00  | 113.86      | 109.39   |
| 7   | C     | 1216 | SGN  | C1-O5-C5 | 3.00  | 116.06      | 112.25   |
| 6   | B     | 1219 | IDS  | C1-O5-C5 | 3.05  | 116.53      | 111.84   |
| 5   | B     | 1212 | SGN  | C1-O5-C5 | 3.08  | 116.16      | 112.25   |
| 8   | F     | 1214 | SGN  | C1-O5-C5 | 3.11  | 116.19      | 112.25   |
| 5   | B     | 1213 | IDS  | C1-O5-C5 | 3.15  | 116.70      | 111.84   |
| 6   | B     | 1220 | SGN  | C1-O5-C5 | 3.18  | 116.28      | 112.25   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 6   | B     | 1222 | SGN  | C1-O5-C5 | 3.19 | 116.30      | 112.25   |
| 5   | B     | 1213 | IDS  | C1-C2-C3 | 3.32 | 114.33      | 109.39   |
| 5   | B     | 1209 | IDS  | O4-C4-C5 | 3.34 | 116.70      | 110.42   |
| 8   | F     | 1211 | IDS  | O4-C4-C5 | 3.36 | 116.75      | 110.42   |
| 5   | B     | 1210 | SGN  | C1-O5-C5 | 3.41 | 116.58      | 112.25   |
| 6   | B     | 1219 | IDS  | C1-C2-C3 | 3.42 | 114.48      | 109.39   |
| 8   | G     | 1213 | SGN  | C1-O5-C5 | 3.47 | 116.65      | 112.25   |
| 7   | C     | 1211 | IDS  | C1-O5-C5 | 3.47 | 117.19      | 111.84   |
| 6   | B     | 1221 | IDS  | C1-C2-C3 | 3.50 | 114.60      | 109.39   |
| 7   | C     | 1213 | IDS  | C1-C2-C3 | 3.54 | 114.66      | 109.39   |
| 7   | C     | 1212 | SGN  | C1-O5-C5 | 3.59 | 116.81      | 112.25   |
| 2   | A     | 1212 | SGN  | O4-C4-C5 | 3.62 | 118.83      | 109.24   |
| 8   | G     | 1210 | IDS  | C1-O5-C5 | 3.67 | 117.50      | 111.84   |
| 2   | A     | 1211 | IDS  | C1-C2-C3 | 3.70 | 114.89      | 109.39   |
| 8   | F     | 1213 | IDS  | C1-C2-C3 | 3.75 | 114.97      | 109.39   |
| 7   | C     | 1211 | IDS  | O4-C4-C3 | 3.89 | 119.08      | 110.34   |
| 8   | F     | 1211 | IDS  | C1-C2-C3 | 3.92 | 115.23      | 109.39   |
| 6   | B     | 1218 | SGN  | C1-O5-C5 | 4.13 | 117.49      | 112.25   |
| 8   | F     | 1214 | SGN  | O4-C4-C5 | 4.37 | 120.82      | 109.24   |
| 8   | G     | 1212 | IDS  | C1-C2-C3 | 4.38 | 115.92      | 109.39   |
| 5   | B     | 1211 | IDS  | C1-C2-C3 | 4.49 | 116.07      | 109.39   |
| 7   | C     | 1212 | SGN  | O4-C4-C5 | 4.75 | 121.84      | 109.24   |
| 2   | A     | 1209 | IDS  | C2-O2-S  | 4.77 | 127.86      | 118.77   |
| 5   | B     | 1214 | SGN  | O4-C4-C5 | 4.82 | 122.00      | 109.24   |
| 6   | B     | 1222 | SGN  | O4-C4-C5 | 4.95 | 122.37      | 109.24   |
| 8   | G     | 1213 | SGN  | O4-C4-C5 | 5.00 | 122.48      | 109.24   |
| 8   | G     | 1210 | IDS  | C1-C2-C3 | 5.08 | 116.95      | 109.39   |
| 7   | C     | 1213 | IDS  | O4-C4-C3 | 5.10 | 121.83      | 110.34   |
| 5   | B     | 1211 | IDS  | O4-C4-C3 | 5.13 | 121.88      | 110.34   |
| 5   | B     | 1209 | IDS  | C2-O2-S  | 5.34 | 128.94      | 118.77   |
| 8   | F     | 1212 | SGN  | O4-C4-C5 | 5.36 | 123.43      | 109.24   |
| 6   | B     | 1217 | IDS  | O4-C4-C3 | 5.53 | 122.78      | 110.34   |
| 7   | C     | 1216 | SGN  | O4-C4-C5 | 5.80 | 124.60      | 109.24   |
| 2   | A     | 1210 | SGN  | O4-C4-C5 | 6.17 | 125.58      | 109.24   |
| 8   | F     | 1213 | IDS  | O4-C4-C5 | 6.78 | 123.18      | 110.42   |
| 8   | G     | 1211 | SGN  | O4-C4-C5 | 6.90 | 127.53      | 109.24   |
| 7   | C     | 1211 | IDS  | O4-C4-C5 | 6.96 | 123.52      | 110.42   |
| 6   | B     | 1217 | IDS  | C2-O2-S  | 8.33 | 134.64      | 118.77   |
| 8   | G     | 1212 | IDS  | O4-C4-C5 | 8.54 | 126.49      | 110.42   |
| 6   | B     | 1221 | IDS  | O4-C4-C5 | 8.76 | 126.90      | 110.42   |
| 5   | B     | 1209 | IDS  | O4-C4-C3 | 8.85 | 130.25      | 110.34   |
| 2   | A     | 1211 | IDS  | O4-C4-C5 | 9.18 | 127.70      | 110.42   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | A     | 1213 | IDS  | O4-C4-C3 | 14.50 | 142.99      | 110.34   |
| 6   | B     | 1223 | IDS  | O4-C4-C3 | 14.87 | 143.81      | 110.34   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 6   | B     | 1223 | IDS  | C4   |
| 2   | A     | 1213 | IDS  | C4   |

All (1) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 6   | B     | 1217 | IDS  | S-O2-C2-C1 |

All (2) ring outliers are listed below:

| Mol | Chain | Res  | Type | Atoms             |
|-----|-------|------|------|-------------------|
| 8   | G     | 1214 | IDS  | C1-C2-C3-C4-C5-O5 |
| 5   | B     | 1215 | IDS  | C1-C2-C3-C4-C5-O5 |

7 monomers are involved in 7 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | B     | 1209 | IDS  | 1       | 0            |
| 6   | B     | 1222 | SGN  | 2       | 0            |
| 6   | B     | 1223 | IDS  | 1       | 0            |
| 6   | B     | 1224 | SGN  | 1       | 0            |
| 7   | C     | 1212 | SGN  | 1       | 0            |
| 7   | C     | 1213 | IDS  | 1       | 0            |
| 8   | F     | 1214 | SGN  | 1       | 0            |

## 5.6 Ligand geometry

16 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 |
| 3   | SO4  | A     | 1215 | -    | 4,4,4        | 3.26 | 2 (50%)  | 6,6,6       | 0.97 | 0        |
| 4   | EPE  | A     | 1216 | -    | 14,15,15     | 1.13 | 1 (7%)   | 18,20,20    | 1.08 | 2 (11%)  |
| 3   | SO4  | B     | 1216 | -    | 4,4,4        | 3.27 | 2 (50%)  | 6,6,6       | 0.96 | 0        |
| 4   | EPE  | B     | 1225 | -    | 14,15,15     | 1.27 | 2 (14%)  | 18,20,20    | 1.14 | 2 (11%)  |
| 3   | SO4  | C     | 1209 | -    | 4,4,4        | 2.90 | 2 (50%)  | 6,6,6       | 1.06 | 0        |
| 4   | EPE  | C     | 1219 | -    | 14,15,15     | 0.94 | 1 (7%)   | 18,20,20    | 1.15 | 2 (11%)  |
| 3   | SO4  | D     | 1209 | -    | 4,4,4        | 3.41 | 2 (50%)  | 6,6,6       | 0.95 | 0        |
| 4   | EPE  | D     | 1210 | -    | 14,15,15     | 1.13 | 1 (7%)   | 18,20,20    | 0.98 | 0        |
| 3   | SO4  | E     | 1210 | -    | 4,4,4        | 3.26 | 2 (50%)  | 6,6,6       | 1.06 | 0        |
| 4   | EPE  | E     | 1211 | -    | 14,15,15     | 1.07 | 1 (7%)   | 18,20,20    | 1.15 | 3 (16%)  |
| 3   | SO4  | F     | 1216 | -    | 4,4,4        | 3.32 | 2 (50%)  | 6,6,6       | 0.96 | 0        |
| 3   | SO4  | F     | 1217 | -    | 4,4,4        | 3.31 | 2 (50%)  | 6,6,6       | 0.95 | 0        |
| 4   | EPE  | F     | 1218 | -    | 14,15,15     | 1.27 | 2 (14%)  | 18,20,20    | 0.82 | 0        |
| 4   | EPE  | G     | 1215 | -    | 14,15,15     | 1.18 | 1 (7%)   | 18,20,20    | 0.96 | 0        |
| 3   | SO4  | H     | 1209 | -    | 4,4,4        | 3.32 | 2 (50%)  | 6,6,6       | 0.97 | 0        |
| 4   | EPE  | H     | 1210 | -    | 14,15,15     | 1.04 | 1 (7%)   | 18,20,20    | 1.04 | 1 (5%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | SO4  | A     | 1215 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | EPE  | A     | 1216 | -    | -       | 0/9/19/19 | 0/1/1/1 |
| 3   | SO4  | B     | 1216 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | EPE  | B     | 1225 | -    | -       | 0/9/19/19 | 0/1/1/1 |
| 3   | SO4  | C     | 1209 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | EPE  | C     | 1219 | -    | -       | 0/9/19/19 | 0/1/1/1 |
| 3   | SO4  | D     | 1209 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | EPE  | D     | 1210 | -    | -       | 0/9/19/19 | 0/1/1/1 |
| 3   | SO4  | E     | 1210 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | EPE  | E     | 1211 | -    | -       | 0/9/19/19 | 0/1/1/1 |
| 3   | SO4  | F     | 1216 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 3   | SO4  | F     | 1217 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | EPE  | F     | 1218 | -    | -       | 0/9/19/19 | 0/1/1/1 |
| 4   | EPE  | G     | 1215 | -    | -       | 0/9/19/19 | 0/1/1/1 |
| 3   | SO4  | H     | 1209 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | EPE  | H     | 1210 | -    | -       | 0/9/19/19 | 0/1/1/1 |

All (26) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | D     | 1209 | SO4  | O3-S  | -4.79 | 1.30        | 1.47     |
| 3   | H     | 1209 | SO4  | O3-S  | -4.76 | 1.30        | 1.47     |
| 3   | B     | 1216 | SO4  | O3-S  | -4.68 | 1.30        | 1.47     |
| 3   | F     | 1217 | SO4  | O3-S  | -4.58 | 1.30        | 1.47     |
| 3   | F     | 1216 | SO4  | O3-S  | -4.55 | 1.31        | 1.47     |
| 3   | A     | 1215 | SO4  | O3-S  | -4.54 | 1.31        | 1.47     |
| 3   | E     | 1210 | SO4  | O3-S  | -4.38 | 1.31        | 1.47     |
| 3   | C     | 1209 | SO4  | O3-S  | -4.16 | 1.32        | 1.47     |
| 4   | C     | 1219 | EPE  | C6-N1 | 2.01  | 1.52        | 1.46     |
| 4   | H     | 1210 | EPE  | C6-N1 | 2.08  | 1.52        | 1.46     |
| 4   | B     | 1225 | EPE  | C6-N1 | 2.19  | 1.52        | 1.46     |
| 4   | B     | 1225 | EPE  | C2-N1 | 2.20  | 1.53        | 1.46     |
| 4   | F     | 1218 | EPE  | C2-N1 | 2.25  | 1.53        | 1.46     |
| 4   | F     | 1218 | EPE  | C6-N1 | 2.29  | 1.53        | 1.46     |
| 4   | G     | 1215 | EPE  | C6-N1 | 2.31  | 1.53        | 1.46     |
| 4   | D     | 1210 | EPE  | C6-N1 | 2.40  | 1.53        | 1.46     |
| 4   | A     | 1216 | EPE  | C6-N1 | 2.45  | 1.53        | 1.46     |
| 4   | E     | 1211 | EPE  | C6-N1 | 2.47  | 1.53        | 1.46     |
| 3   | C     | 1209 | SO4  | O1-S  | 3.95  | 1.60        | 1.47     |
| 3   | B     | 1216 | SO4  | O1-S  | 4.37  | 1.62        | 1.47     |
| 3   | H     | 1209 | SO4  | O1-S  | 4.49  | 1.62        | 1.47     |
| 3   | A     | 1215 | SO4  | O1-S  | 4.56  | 1.62        | 1.47     |
| 3   | D     | 1209 | SO4  | O1-S  | 4.64  | 1.63        | 1.47     |
| 3   | F     | 1217 | SO4  | O1-S  | 4.68  | 1.63        | 1.47     |
| 3   | F     | 1216 | SO4  | O1-S  | 4.71  | 1.63        | 1.47     |
| 3   | E     | 1210 | SO4  | O1-S  | 4.73  | 1.63        | 1.47     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4   | B     | 1225 | EPE  | O1S-S-C10 | -2.79 | 104.52      | 106.91   |
| 4   | H     | 1210 | EPE  | O1S-S-C10 | -2.70 | 104.60      | 106.91   |
| 4   | C     | 1219 | EPE  | O1S-S-C10 | -2.27 | 104.96      | 106.91   |
| 4   | E     | 1211 | EPE  | O1S-S-C10 | -2.25 | 104.99      | 106.91   |
| 4   | E     | 1211 | EPE  | C3-C2-N1  | -2.23 | 106.63      | 110.63   |
| 4   | A     | 1216 | EPE  | C3-C2-N1  | -2.09 | 106.89      | 110.63   |
| 4   | E     | 1211 | EPE  | C7-N4-C5  | -2.08 | 105.94      | 111.27   |
| 4   | A     | 1216 | EPE  | C7-N4-C5  | -2.04 | 106.03      | 111.27   |
| 4   | C     | 1219 | EPE  | O2S-S-C10 | 2.01  | 108.62      | 106.91   |
| 4   | B     | 1225 | EPE  | O2S-S-C10 | 2.36  | 108.92      | 106.91   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1216 | EPE  | 1       | 0            |
| 4   | B     | 1225 | EPE  | 2       | 0            |
| 3   | C     | 1209 | SO4  | 2       | 0            |
| 4   | C     | 1219 | EPE  | 3       | 0            |
| 3   | D     | 1209 | SO4  | 1       | 0            |
| 4   | D     | 1210 | EPE  | 1       | 0            |
| 4   | E     | 1211 | EPE  | 1       | 0            |
| 3   | F     | 1216 | SO4  | 2       | 0            |
| 4   | F     | 1218 | EPE  | 1       | 0            |
| 3   | H     | 1209 | SO4  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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     | 172/183 (93%)   | 0.05   | 7 (4%) 41 16  | 22, 50, 91, 102       | 0     |
| 1   | B     | 172/183 (93%)   | -0.21  | 1 (0%) 90 73  | 18, 47, 84, 94        | 0     |
| 1   | C     | 172/183 (93%)   | -0.36  | 0 100 100     | 10, 35, 55, 72        | 0     |
| 1   | D     | 172/183 (93%)   | -0.13  | 1 (0%) 90 73  | 17, 48, 87, 90        | 0     |
| 1   | E     | 173/183 (94%)   | -0.01  | 2 (1%) 81 55  | 22, 54, 88, 98        | 0     |
| 1   | F     | 173/183 (94%)   | -0.11  | 3 (1%) 73 45  | 18, 49, 92, 109       | 0     |
| 1   | G     | 164/183 (89%)   | 0.31   | 7 (4%) 39 16  | 43, 69, 95, 103       | 0     |
| 1   | H     | 171/183 (93%)   | 0.28   | 13 (7%) 17 6  | 24, 65, 114, 129      | 0     |
| All | All   | 1369/1464 (93%) | -0.03  | 34 (2%) 61 30 | 10, 52, 94, 129       | 0     |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 66  | THR  | 4.0  |
| 1   | F     | 209 | VAL  | 3.5  |
| 1   | H     | 65  | ASN  | 3.2  |
| 1   | A     | 57  | LEU  | 3.1  |
| 1   | H     | 107 | GLY  | 3.0  |
| 1   | A     | 96  | CYS  | 3.0  |
| 1   | G     | 65  | ASN  | 2.9  |
| 1   | F     | 56  | ALA  | 2.9  |
| 1   | G     | 112 | PHE  | 2.9  |
| 1   | B     | 56  | ALA  | 2.8  |
| 1   | H     | 88  | VAL  | 2.7  |
| 1   | A     | 65  | ASN  | 2.6  |
| 1   | A     | 90  | ASP  | 2.6  |
| 1   | D     | 96  | CYS  | 2.5  |
| 1   | G     | 108 | VAL  | 2.4  |
| 1   | A     | 114 | HIS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 72  | ASP  | 2.4  |
| 1   | G     | 96  | CYS  | 2.4  |
| 1   | H     | 57  | LEU  | 2.4  |
| 1   | H     | 106 | SER  | 2.3  |
| 1   | G     | 70  | CYS  | 2.3  |
| 1   | H     | 70  | CYS  | 2.3  |
| 1   | H     | 91  | LYS  | 2.3  |
| 1   | G     | 156 | ILE  | 2.3  |
| 1   | A     | 56  | ALA  | 2.2  |
| 1   | H     | 56  | ALA  | 2.2  |
| 1   | E     | 98  | TRP  | 2.2  |
| 1   | G     | 40  | HIS  | 2.2  |
| 1   | H     | 59  | ILE  | 2.2  |
| 1   | H     | 114 | HIS  | 2.2  |
| 1   | H     | 72  | ASP  | 2.1  |
| 1   | H     | 208 | GLU  | 2.0  |
| 1   | A     | 54  | ASP  | 2.0  |
| 1   | E     | 107 | GLY  | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 5   | SGN  | B     | 1210 | 19/20 | 0.69 | 0.42 | 3.82 | 138,141,143,143            | 0     |
| 7   | SGN  | C     | 1212 | 19/20 | 0.81 | 0.30 | 3.52 | 94,101,106,106             | 0     |
| 2   | SGN  | A     | 1210 | 19/20 | 0.69 | 0.34 | 2.07 | 120,121,124,124            | 0     |
| 8   | SGN  | G     | 1213 | 19/20 | 0.64 | 0.43 | 1.55 | 125,126,129,129            | 0     |
| 2   | SGN  | A     | 1212 | 19/20 | 0.74 | 0.46 | 1.46 | 123,125,127,127            | 0     |
| 8   | IDS  | G     | 1212 | 16/17 | 0.77 | 0.31 | 0.58 | 123,124,126,127            | 0     |
| 6   | SGN  | B     | 1218 | 19/20 | 0.88 | 0.21 | 0.36 | 95,103,105,105             | 0     |
| 8   | IDS  | F     | 1215 | 15/17 | 0.78 | 0.30 | 0.27 | 127,130,132,132            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 2   | IDS  | A     | 1211 | 16/17 | 0.71 | 0.29 | -0.05 | 118,121,122,122             | 0     |
| 7   | SGN  | C     | 1216 | 19/20 | 0.92 | 0.18 | -0.75 | 75,79,81,89                 | 0     |
| 6   | SGN  | B     | 1220 | 19/20 | 0.90 | 0.22 | -0.81 | 70,79,82,89                 | 0     |
| 6   | IDS  | B     | 1221 | 16/17 | 0.88 | 0.18 | -1.10 | 93,97,102,102               | 0     |
| 5   | IDS  | B     | 1209 | 17/17 | 0.61 | 0.47 | -     | 142,145,146,146             | 0     |
| 8   | IDS  | G     | 1210 | 16/17 | 0.72 | 0.39 | -     | 122,129,131,131             | 0     |
| 8   | IDS  | F     | 1213 | 16/17 | 0.85 | 0.26 | -     | 134,135,136,137             | 0     |
| 6   | IDS  | B     | 1219 | 16/17 | 0.89 | 0.26 | -     | 82,90,92,93                 | 0     |
| 8   | SGN  | F     | 1212 | 19/20 | 0.81 | 0.24 | -     | 127,131,132,133             | 0     |
| 5   | IDS  | B     | 1213 | 16/17 | 0.76 | 0.45 | -     | 139,140,141,144             | 0     |
| 6   | IDS  | B     | 1217 | 17/17 | 0.75 | 0.34 | -     | 106,114,118,118             | 0     |
| 8   | SGN  | G     | 1211 | 19/20 | 0.84 | 0.18 | -     | 119,120,121,122             | 0     |
| 7   | IDS  | C     | 1215 | 16/17 | 0.93 | 0.14 | -     | 76,78,82,82                 | 0     |
| 8   | SGN  | F     | 1210 | 20/20 | 0.56 | 0.50 | -     | 143,150,155,155             | 0     |
| 5   | IDS  | B     | 1215 | 15/17 | 0.77 | 0.48 | -     | 144,144,145,145             | 0     |
| 7   | IDS  | C     | 1211 | 16/17 | 0.80 | 0.27 | -     | 103,106,106,106             | 0     |
| 7   | SGN  | C     | 1210 | 20/20 | 0.71 | 0.22 | -     | 105,112,122,122             | 0     |
| 5   | IDS  | B     | 1211 | 16/17 | 0.56 | 0.42 | -     | 138,140,142,142             | 0     |
| 2   | IDS  | A     | 1209 | 17/17 | 0.74 | 0.49 | -     | 121,122,123,123             | 0     |
| 6   | IDS  | B     | 1223 | 16/17 | 0.83 | 0.28 | -     | 106,112,115,123             | 0     |
| 6   | SGN  | B     | 1224 | 18/20 | 0.77 | 0.34 | -     | 124,127,129,129             | 0     |
| 2   | SGN  | A     | 1214 | 18/20 | 0.62 | 0.43 | -     | 132,134,142,142             | 0     |
| 7   | IDS  | C     | 1217 | 16/17 | 0.91 | 0.17 | -     | 90,95,101,114               | 0     |
| 8   | SGN  | G     | 1209 | 20/20 | 0.65 | 0.50 | -     | 131,137,140,140             | 0     |
| 2   | IDS  | A     | 1213 | 16/17 | 0.82 | 0.36 | -     | 125,127,130,131             | 0     |
| 7   | IDS  | C     | 1213 | 16/17 | 0.83 | 0.19 | -     | 71,87,89,91                 | 0     |
| 5   | SGN  | B     | 1214 | 19/20 | 0.69 | 0.41 | -     | 143,145,146,147             | 0     |
| 7   | SGN  | C     | 1218 | 18/20 | 0.67 | 0.38 | -     | 118,126,130,130             | 0     |
| 5   | SGN  | B     | 1212 | 19/20 | 0.79 | 0.25 | -     | 134,137,138,138             | 0     |
| 7   | SGN  | C     | 1214 | 19/20 | 0.89 | 0.20 | -     | 55,60,67,74                 | 0     |
| 8   | IDS  | F     | 1211 | 16/17 | 0.62 | 0.45 | -     | 134,140,143,143             | 0     |
| 8   | SGN  | F     | 1214 | 19/20 | 0.76 | 0.32 | -     | 132,135,137,137             | 0     |
| 6   | SGN  | B     | 1222 | 19/20 | 0.84 | 0.20 | -     | 97,103,107,109              | 0     |
| 8   | IDS  | G     | 1214 | 15/17 | 0.75 | 0.44 | -     | 125,125,126,127             | 0     |

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 4   | EPE  | F     | 1218 | 15/15 | 0.78 | 0.41 | 4.85  | 102,103,104,105             | 0     |
| 3   | SO4  | A     | 1215 | 5/5   | 0.88 | 0.27 | 2.34  | 126,126,127,127             | 0     |
| 4   | EPE  | C     | 1219 | 15/15 | 0.93 | 0.26 | 1.47  | 46,50,53,53                 | 0     |
| 4   | EPE  | E     | 1211 | 15/15 | 0.93 | 0.24 | 1.28  | 64,69,70,70                 | 0     |
| 3   | SO4  | F     | 1217 | 5/5   | 0.91 | 0.26 | 1.10  | 133,133,133,134             | 0     |
| 3   | SO4  | C     | 1209 | 5/5   | 0.90 | 0.22 | 0.72  | 108,108,109,110             | 0     |
| 4   | EPE  | A     | 1216 | 15/15 | 0.95 | 0.20 | 0.61  | 35,37,43,44                 | 0     |
| 4   | EPE  | G     | 1215 | 15/15 | 0.90 | 0.28 | 0.49  | 73,80,86,86                 | 0     |
| 4   | EPE  | D     | 1210 | 15/15 | 0.93 | 0.20 | 0.18  | 62,67,68,68                 | 0     |
| 3   | SO4  | D     | 1209 | 5/5   | 0.94 | 0.21 | 0.04  | 102,102,102,103             | 0     |
| 4   | EPE  | B     | 1225 | 15/15 | 0.95 | 0.18 | -0.34 | 35,46,53,53                 | 0     |
| 3   | SO4  | E     | 1210 | 5/5   | 0.94 | 0.17 | -0.42 | 94,94,95,95                 | 0     |
| 3   | SO4  | B     | 1216 | 5/5   | 0.95 | 0.15 | -0.55 | 101,101,101,101             | 0     |
| 3   | SO4  | F     | 1216 | 5/5   | 0.93 | 0.17 | -0.60 | 111,112,112,112             | 0     |
| 3   | SO4  | H     | 1209 | 5/5   | 0.95 | 0.14 | -0.67 | 82,83,83,83                 | 0     |
| 4   | EPE  | H     | 1210 | 15/15 | 0.95 | 0.16 | -0.74 | 54,55,57,58                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.