



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:51 PM UTC

PDB ID : 5OCD / pdb\_00005ocd  
Title : structure of a CDPS from *Fluoribacter dumoffii*  
Authors : Schmitt, E.; Mechulam, Y.; Bourgeois, G.  
Deposited on : 2017-06-30  
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

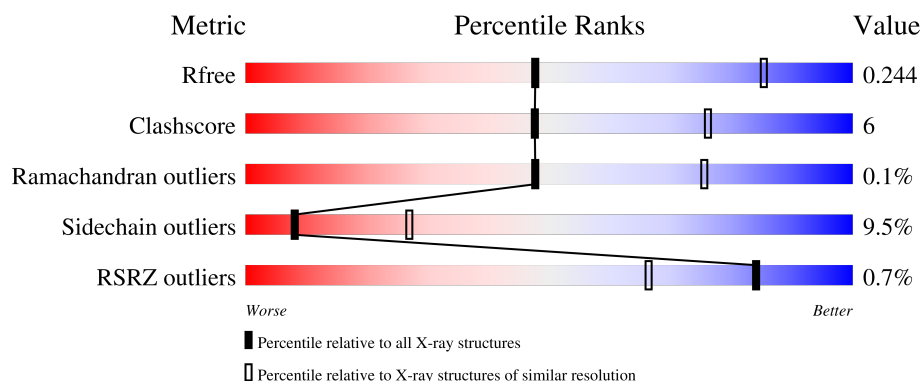
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2469 (3.10-3.02)                                      |
| Clashscore            | 190562                      | 2569 (3.10-3.02)                                      |
| Ramachandran outliers | 187476                      | 2424 (3.10-3.02)                                      |
| Sidechain outliers    | 187428                      | 2423 (3.10-3.02)                                      |
| RSRZ outliers         | 180081                      | 2469 (3.10-3.02)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                          |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------------|
| 1   | A     | 266    | <br>62% 20% 15% 3% 2% |
| 1   | B     | 266    | <br>64% 18% 15% 1% 1% |
| 1   | C     | 266    | <br>67% 15% 15% 1% 1% |
| 1   | D     | 266    | <br>65% 17% 15% 1% 1% |
| 1   | E     | 266    | <br>62% 20% 16% 1% 1% |

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| Mol | Chain | Length | Quality of chain                                                                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | F     | 266    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>59%</div><div>20%</div><div>• •</div><div>17%</div></div> |
| 1   | G     | 266    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>61%</div><div>18%</div><div>•</div><div>17%</div></div>                |
| 1   | H     | 266    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div>65%</div><div>16%</div><div>•</div><div>15%</div></div>    |
| 1   | I     | 266    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>66%</div><div>15%</div><div>•</div><div>16%</div></div>                |
| 1   | J     | 266    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div>64%</div><div>17%</div><div>•</div><div>16%</div></div>    |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18821 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 Cyclodipeptide synthase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1893  | 1212 | 329 | 342 | 10 |         |         |       |
| 1   | B     | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1893  | 1212 | 329 | 342 | 10 |         |         |       |
| 1   | C     | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1892  | 1213 | 328 | 341 | 10 |         |         |       |
| 1   | D     | 225      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1885  | 1208 | 327 | 340 | 10 |         |         |       |
| 1   | E     | 224      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1204 | 327 | 339 | 10 |         |         |       |
| 1   | F     | 220      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1842  | 1181 | 319 | 332 | 10 |         |         |       |
| 1   | G     | 221      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1846  | 1184 | 317 | 335 | 10 |         |         |       |
| 1   | H     | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1886  | 1210 | 325 | 341 | 10 |         |         |       |
| 1   | I     | 224      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1874  | 1202 | 323 | 339 | 10 |         |         |       |
| 1   | J     | 224      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1874  | 1202 | 323 | 339 | 10 |         |         |       |

There are 100 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference      |
|-------|---------|----------|--------|-----------------------|----------------|
| A     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| A     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| A     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| A     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| A     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| A     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| A     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| A     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| A     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference      |
|-------|---------|----------|--------|-----------------------|----------------|
| A     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| B     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| B     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| C     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| C     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| D     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| D     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| E     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| E     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference      |
|-------|---------|----------|--------|-----------------------|----------------|
| F     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| F     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| G     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| G     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| H     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| H     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| I     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 259     | ARG      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 260     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 261     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 262     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 263     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 264     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| I     | 265     | HIS      | -      | expression tag        | UNP A0A0W0T5C6 |
| J     | 0       | MET      | -      | initiating methionine | UNP A0A0W0T5C6 |
| J     | 1       | ALA      | -      | expression tag        | UNP A0A0W0T5C6 |
| J     | 258     | SER      | -      | expression tag        | UNP A0A0W0T5C6 |

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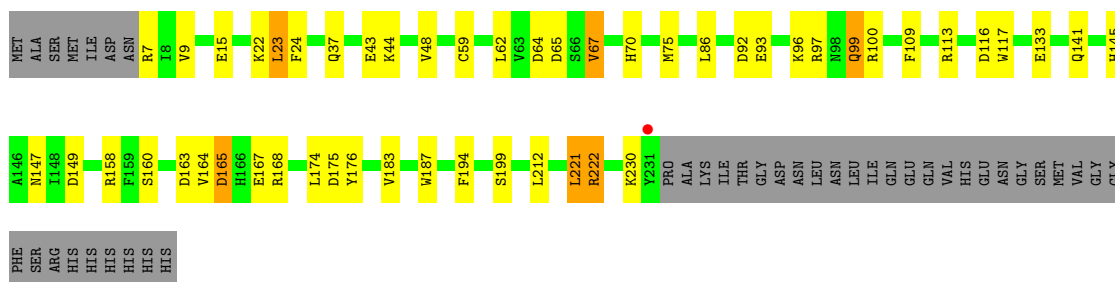
| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| J     | 259     | ARG      | -      | expression tag | UNP A0A0W0T5C6 |
| J     | 260     | HIS      | -      | expression tag | UNP A0A0W0T5C6 |
| J     | 261     | HIS      | -      | expression tag | UNP A0A0W0T5C6 |
| J     | 262     | HIS      | -      | expression tag | UNP A0A0W0T5C6 |
| J     | 263     | HIS      | -      | expression tag | UNP A0A0W0T5C6 |
| J     | 264     | HIS      | -      | expression tag | UNP A0A0W0T5C6 |
| J     | 265     | HIS      | -      | expression tag | UNP A0A0W0T5C6 |

- Molecule 2 is water.

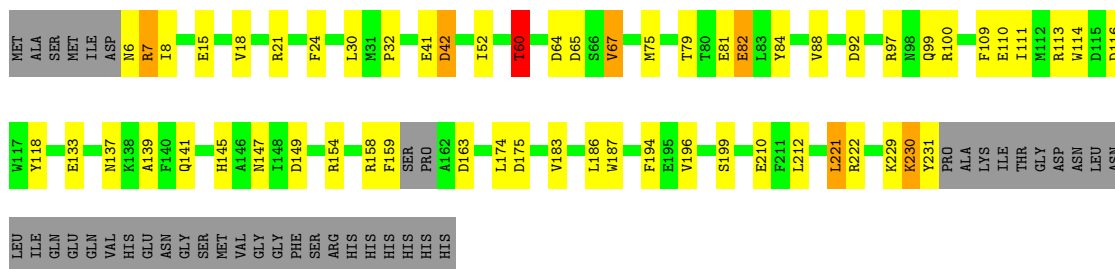
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2   | A     | 15       | Total O<br>15 15 | 0       | 0       |
| 2   | B     | 8        | Total O<br>8 8   | 0       | 0       |
| 2   | C     | 5        | Total O<br>5 5   | 0       | 0       |
| 2   | D     | 9        | Total O<br>9 9   | 0       | 0       |
| 2   | E     | 1        | Total O<br>1 1   | 0       | 0       |
| 2   | F     | 1        | Total O<br>1 1   | 0       | 0       |
| 2   | G     | 1        | Total O<br>1 1   | 0       | 0       |
| 2   | H     | 4        | Total O<br>4 4   | 0       | 0       |
| 2   | I     | 5        | Total O<br>5 5   | 0       | 0       |
| 2   | J     | 7        | Total O<br>7 7   | 0       | 0       |



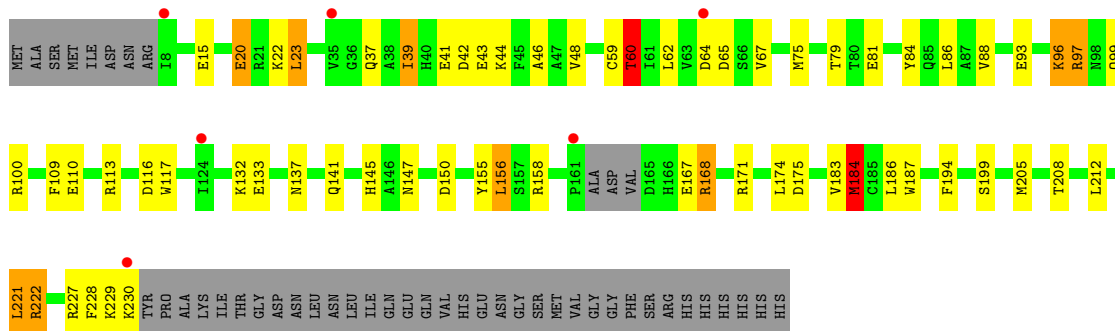
Chain D:  65% 17% • 15%



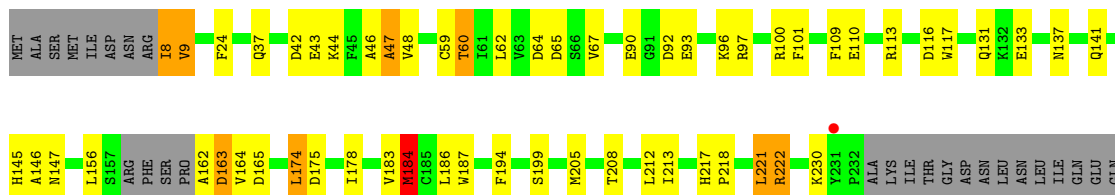
Chain E:  62% 20% • 16%



Chain F: 



Chain G:  61% 18% • 17%



VAL  
HIS  
GLU  
SER  
ASN  
GLY  
ILE  
SER  
MET  
VAL  
GLY  
PHE  
SER  
ARG  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 1: Cyclodipectase synthase

Chain H:  65% 16% 15%

MET ALA SER MET ILE ASP ASN ARG 18 V9 V18 V19 E20 R21 K22 P25 V35 E43 K44 F45 V48 V49 C59 T60 T61 L62 V63 D64 D65 S66 V67 M75 T79 E82 E90 G91 D92 E93 K96 Q99 F109 E110 R113 D116 W117

I124 H127 E133 N137 Q141 H145 A146 N147 I148 D149 D150 R154 R158 D163 L174 D175 V183 M184 W187 F194 S199 K205 T208 L212 L221 R222 A233 LYS ILE THR ASP ASN LEU LEU ILE GLN GLU VAL

HIS GLU ASN GLY SER MET VAL GLY PHE ARG HIS HIS HIS HIS HIS HIS

• Molecule 1: Cyclodipectase synthase

Chain I:  66% 15% 16%

MET ALA SER MET ILE ASP ASN ARG 18 L23 F24 D42 E43 K44 V48 C59 T60 T61 L62 V63 D64 D65 S66 V67 M75 D92 E93 K96 R97 N98 Q99 R100 F109 E110 R113 D116 W117 E133 N137 Q141 H145 A146 N147 I148 D150

R158 S160 D163 L174 D175 V183 L186 W187 F194 E195 S199 G200 R201 L212 L221 R222 Y231 PRO ALA LYS ILE THR GLY ASP ASN LEU ASN ILE LEU GLN GLU VAL HIS GLU ASN GLY SER MET VAL GLY PHE SER ARG HIS HIS HIS

HIS HIS

• Molecule 1: Cyclodipectase synthase

Chain J:  64% 17% 16%

MET ALA SER MET ILE ASP ASN ARG 18 V9 R14 E15 K22 L23 F24 H40 E41 E42 E43 F45 C59 T60 T61 L62 V63 D64 D65 S66 V67 M75 Q85 L86 K89 D92 R97 N98 Q99 R100 F109 E110 R113 W114 D115 D116 W117 Y123 I124

N125 S126 E133 Q141 H145 D150 F159 S160 P161 A162 D163 L174 D175 V183 W187 F194 S199 L212 L221 R222 K229 K230 Y231 PRO ALA LYS ILE THR GLY ASP ASN LEU ASN ILE GLN GLU VAL HIS GLU GLY SER MET VAL GLY

GLY PHE SER ARG HIS HIS HIS HIS HIS

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 185.03Å 97.80Å 211.28Å<br>90.00° 115.58° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 48.16 – 3.06<br>48.16 – 3.06                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (48.16-3.06)<br>99.3 (48.16-3.06)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.33 (at 3.07Å)                                             | Xtriage          |
| Refinement program                                                      | BUSTER 2.10.3                                               | Depositor        |
| R, $R_{free}$                                                           | 0.210 , 0.249<br>0.217 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3223 reflections (4.99%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.894                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 60.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for h,-k,-h-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 18821                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 94.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5771e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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     | 0.97         | 2/1943 (0.1%)  | 1.42        | 14/2629 (0.5%)   |
| 1   | B     | 0.90         | 0/1943         | 1.43        | 15/2629 (0.6%)   |
| 1   | C     | 0.84         | 1/1943 (0.1%)  | 1.41        | 11/2630 (0.4%)   |
| 1   | D     | 0.86         | 0/1935         | 1.39        | 15/2618 (0.6%)   |
| 1   | E     | 0.91         | 0/1928         | 1.45        | 16/2606 (0.6%)   |
| 1   | F     | 0.83         | 1/1890 (0.1%)  | 1.43        | 23/2555 (0.9%)   |
| 1   | G     | 0.82         | 1/1894 (0.1%)  | 1.46        | 21/2563 (0.8%)   |
| 1   | H     | 0.82         | 0/1937         | 1.42        | 18/2623 (0.7%)   |
| 1   | I     | 0.81         | 0/1924         | 1.40        | 16/2604 (0.6%)   |
| 1   | J     | 0.86         | 0/1924         | 1.47        | 21/2604 (0.8%)   |
| All | All   | 0.86         | 5/19261 (0.0%) | 1.43        | 170/26061 (0.7%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 184 | MET  | SD-CE | -7.58 | 1.60        | 1.79     |
| 1   | C     | 184 | MET  | SD-CE | -6.50 | 1.63        | 1.79     |
| 1   | A     | 197 | TYR  | CA-C  | 5.72  | 1.57        | 1.52     |
| 1   | G     | 184 | MET  | SD-CE | -5.57 | 1.65        | 1.79     |
| 1   | F     | 184 | MET  | SD-CE | -5.34 | 1.66        | 1.79     |

All (170) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 65  | ASP  | CA-CB-CG | 10.22 | 122.82      | 112.60   |
| 1   | B     | 65  | ASP  | CA-CB-CG | 8.78  | 121.38      | 112.60   |
| 1   | G     | 163 | ASP  | CA-C-N   | 7.51  | 132.06      | 122.37   |
| 1   | G     | 163 | ASP  | C-N-CA   | 7.51  | 132.06      | 122.37   |
| 1   | E     | 64  | ASP  | CA-CB-CG | 7.39  | 119.99      | 112.60   |
| 1   | A     | 92  | ASP  | CA-CB-CG | 7.01  | 119.61      | 112.60   |
| 1   | I     | 64  | ASP  | CA-CB-CG | 7.01  | 119.61      | 112.60   |
| 1   | H     | 64  | ASP  | CA-CB-CG | 6.94  | 119.54      | 112.60   |
| 1   | C     | 64  | ASP  | CA-CB-CG | 6.88  | 119.48      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 92  | ASP  | CA-CB-CG | 6.82  | 119.42      | 112.60   |
| 1   | J     | 92  | ASP  | CA-CB-CG | 6.71  | 119.31      | 112.60   |
| 1   | C     | 92  | ASP  | CA-CB-CG | 6.70  | 119.30      | 112.60   |
| 1   | D     | 64  | ASP  | CA-CB-CG | 6.67  | 119.28      | 112.60   |
| 1   | E     | 163 | ASP  | CA-C-N   | 6.67  | 129.63      | 120.35   |
| 1   | E     | 163 | ASP  | C-N-CA   | 6.67  | 129.63      | 120.35   |
| 1   | I     | 42  | ASP  | CA-C-N   | 6.54  | 130.63      | 120.82   |
| 1   | I     | 42  | ASP  | C-N-CA   | 6.54  | 130.63      | 120.82   |
| 1   | F     | 64  | ASP  | CA-CB-CG | 6.54  | 119.14      | 112.60   |
| 1   | G     | 165 | ASP  | N-CA-C   | -6.53 | 100.50      | 109.71   |
| 1   | H     | 92  | ASP  | CA-CB-CG | 6.50  | 119.10      | 112.60   |
| 1   | H     | 22  | LYS  | CA-C-N   | 6.48  | 129.49      | 120.29   |
| 1   | H     | 22  | LYS  | C-N-CA   | 6.48  | 129.49      | 120.29   |
| 1   | D     | 92  | ASP  | CA-CB-CG | 6.46  | 119.06      | 112.60   |
| 1   | G     | 92  | ASP  | CA-CB-CG | 6.42  | 119.02      | 112.60   |
| 1   | E     | 92  | ASP  | CA-CB-CG | 6.42  | 119.02      | 112.60   |
| 1   | I     | 92  | ASP  | CA-CB-CG | 6.37  | 118.97      | 112.60   |
| 1   | E     | 60  | THR  | CB-CA-C  | 6.32  | 119.03      | 110.94   |
| 1   | J     | 64  | ASP  | CA-CB-CG | 6.22  | 118.82      | 112.60   |
| 1   | B     | 175 | ASP  | CA-CB-CG | 6.19  | 118.79      | 112.60   |
| 1   | D     | 99  | GLN  | CA-C-N   | 6.16  | 128.82      | 120.38   |
| 1   | D     | 99  | GLN  | C-N-CA   | 6.16  | 128.82      | 120.38   |
| 1   | H     | 175 | ASP  | CA-CB-CG | 6.10  | 118.70      | 112.60   |
| 1   | A     | 99  | GLN  | CA-C-N   | 6.08  | 128.71      | 120.38   |
| 1   | A     | 99  | GLN  | C-N-CA   | 6.08  | 128.71      | 120.38   |
| 1   | G     | 64  | ASP  | CA-CB-CG | 6.07  | 118.67      | 112.60   |
| 1   | E     | 116 | ASP  | CA-CB-CG | 6.04  | 118.64      | 112.60   |
| 1   | G     | 116 | ASP  | CA-CB-CG | 5.98  | 118.58      | 112.60   |
| 1   | I     | 99  | GLN  | CA-C-N   | 5.93  | 128.50      | 120.38   |
| 1   | I     | 99  | GLN  | C-N-CA   | 5.93  | 128.50      | 120.38   |
| 1   | E     | 139 | ALA  | CA-C-N   | 5.93  | 128.50      | 120.44   |
| 1   | E     | 139 | ALA  | C-N-CA   | 5.93  | 128.50      | 120.44   |
| 1   | C     | 65  | ASP  | CA-CB-CG | 5.91  | 118.51      | 112.60   |
| 1   | H     | 96  | LYS  | CA-C-N   | 5.90  | 128.51      | 120.54   |
| 1   | H     | 96  | LYS  | C-N-CA   | 5.90  | 128.51      | 120.54   |
| 1   | G     | 65  | ASP  | CA-CB-CG | 5.88  | 118.48      | 112.60   |
| 1   | B     | 99  | GLN  | CA-C-N   | 5.83  | 128.37      | 120.38   |
| 1   | B     | 99  | GLN  | C-N-CA   | 5.83  | 128.37      | 120.38   |
| 1   | J     | 42  | ASP  | CA-C-N   | 5.82  | 129.56      | 120.82   |
| 1   | J     | 42  | ASP  | C-N-CA   | 5.82  | 129.56      | 120.82   |
| 1   | A     | 199 | SER  | CA-C-N   | -5.80 | 113.96      | 121.96   |
| 1   | A     | 199 | SER  | C-N-CA   | -5.80 | 113.96      | 121.96   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 116 | ASP  | CA-CB-CG | 5.78  | 118.38      | 112.60   |
| 1   | J     | 65  | ASP  | CA-CB-CG | 5.76  | 118.36      | 112.60   |
| 1   | E     | 65  | ASP  | CA-CB-CG | 5.76  | 118.36      | 112.60   |
| 1   | B     | 42  | ASP  | CA-C-N   | 5.74  | 129.42      | 120.82   |
| 1   | B     | 42  | ASP  | C-N-CA   | 5.74  | 129.42      | 120.82   |
| 1   | F     | 20  | GLU  | CA-C-N   | 5.71  | 128.50      | 120.28   |
| 1   | F     | 20  | GLU  | C-N-CA   | 5.71  | 128.50      | 120.28   |
| 1   | H     | 99  | GLN  | CA-C-N   | 5.70  | 128.19      | 120.38   |
| 1   | H     | 99  | GLN  | C-N-CA   | 5.70  | 128.19      | 120.38   |
| 1   | H     | 65  | ASP  | CA-CB-CG | 5.68  | 118.28      | 112.60   |
| 1   | E     | 175 | ASP  | CA-CB-CG | 5.67  | 118.27      | 112.60   |
| 1   | C     | 24  | PHE  | CA-CB-CG | 5.65  | 119.45      | 113.80   |
| 1   | I     | 116 | ASP  | CA-CB-CG | 5.65  | 118.25      | 112.60   |
| 1   | B     | 67  | VAL  | CB-CA-C  | -5.64 | 104.53      | 112.14   |
| 1   | B     | 116 | ASP  | CA-CB-CG | 5.63  | 118.23      | 112.60   |
| 1   | H     | 21  | ARG  | CA-C-N   | 5.63  | 128.13      | 120.54   |
| 1   | H     | 21  | ARG  | C-N-CA   | 5.63  | 128.13      | 120.54   |
| 1   | B     | 36  | GLY  | N-CA-C   | 5.61  | 120.58      | 113.24   |
| 1   | D     | 65  | ASP  | CA-CB-CG | 5.60  | 118.20      | 112.60   |
| 1   | D     | 149 | ASP  | CA-CB-CG | 5.60  | 118.20      | 112.60   |
| 1   | A     | 175 | ASP  | CA-CB-CG | 5.59  | 118.19      | 112.60   |
| 1   | E     | 24  | PHE  | CA-CB-CG | 5.58  | 119.38      | 113.80   |
| 1   | H     | 150 | ASP  | CA-CB-CG | 5.56  | 118.16      | 112.60   |
| 1   | J     | 159 | PHE  | CA-C-N   | 5.56  | 128.12      | 120.39   |
| 1   | J     | 159 | PHE  | C-N-CA   | 5.56  | 128.12      | 120.39   |
| 1   | J     | 230 | LYS  | CA-C-N   | 5.55  | 131.69      | 121.70   |
| 1   | J     | 230 | LYS  | C-N-CA   | 5.55  | 131.69      | 121.70   |
| 1   | J     | 116 | ASP  | CA-CB-CG | 5.54  | 118.14      | 112.60   |
| 1   | E     | 82  | GLU  | CA-C-N   | 5.52  | 127.68      | 120.28   |
| 1   | E     | 82  | GLU  | C-N-CA   | 5.52  | 127.68      | 120.28   |
| 1   | I     | 96  | LYS  | CA-C-N   | 5.51  | 127.98      | 120.54   |
| 1   | I     | 96  | LYS  | C-N-CA   | 5.51  | 127.98      | 120.54   |
| 1   | F     | 65  | ASP  | CA-CB-CG | 5.51  | 118.11      | 112.60   |
| 1   | I     | 65  | ASP  | CA-CB-CG | 5.49  | 118.09      | 112.60   |
| 1   | F     | 175 | ASP  | CA-CB-CG | 5.48  | 118.08      | 112.60   |
| 1   | C     | 175 | ASP  | CA-CB-CG | 5.47  | 118.07      | 112.60   |
| 1   | B     | 150 | ASP  | CA-CB-CG | 5.47  | 118.07      | 112.60   |
| 1   | B     | 37  | GLN  | CA-C-N   | 5.46  | 128.61      | 120.31   |
| 1   | B     | 37  | GLN  | C-N-CA   | 5.46  | 128.61      | 120.31   |
| 1   | A     | 96  | LYS  | CA-C-N   | 5.44  | 127.84      | 120.38   |
| 1   | A     | 96  | LYS  | C-N-CA   | 5.44  | 127.84      | 120.38   |
| 1   | I     | 175 | ASP  | CA-CB-CG | 5.44  | 118.04      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 43  | GLU  | CA-C-N   | 5.42  | 127.49      | 120.44   |
| 1   | F     | 43  | GLU  | C-N-CA   | 5.42  | 127.49      | 120.44   |
| 1   | F     | 46  | ALA  | CA-C-N   | 5.39  | 127.45      | 120.44   |
| 1   | F     | 46  | ALA  | C-N-CA   | 5.39  | 127.45      | 120.44   |
| 1   | A     | 150 | ASP  | CA-CB-CG | 5.39  | 117.99      | 112.60   |
| 1   | J     | 175 | ASP  | CA-CB-CG | 5.37  | 117.97      | 112.60   |
| 1   | E     | 137 | ASN  | CA-CB-CG | 5.37  | 117.97      | 112.60   |
| 1   | G     | 47  | ALA  | CA-C-N   | 5.36  | 127.42      | 120.56   |
| 1   | G     | 47  | ALA  | C-N-CA   | 5.36  | 127.42      | 120.56   |
| 1   | D     | 165 | ASP  | CA-CB-CG | 5.34  | 117.94      | 112.60   |
| 1   | D     | 37  | GLN  | CA-C-N   | 5.31  | 128.38      | 120.31   |
| 1   | D     | 37  | GLN  | C-N-CA   | 5.31  | 128.38      | 120.31   |
| 1   | G     | 37  | GLN  | CA-C-N   | 5.31  | 128.38      | 120.31   |
| 1   | G     | 37  | GLN  | C-N-CA   | 5.31  | 128.38      | 120.31   |
| 1   | J     | 161 | PRO  | CA-C-N   | 5.30  | 127.39      | 120.28   |
| 1   | J     | 161 | PRO  | C-N-CA   | 5.30  | 127.39      | 120.28   |
| 1   | C     | 116 | ASP  | CA-CB-CG | 5.30  | 117.90      | 112.60   |
| 1   | I     | 137 | ASN  | CA-CB-CG | 5.28  | 117.88      | 112.60   |
| 1   | H     | 116 | ASP  | CA-CB-CG | 5.28  | 117.88      | 112.60   |
| 1   | G     | 146 | ALA  | CA-C-N   | 5.25  | 127.31      | 120.28   |
| 1   | G     | 146 | ALA  | C-N-CA   | 5.25  | 127.31      | 120.28   |
| 1   | J     | 123 | TYR  | CA-C-N   | 5.24  | 127.64      | 120.77   |
| 1   | J     | 123 | TYR  | C-N-CA   | 5.24  | 127.64      | 120.77   |
| 1   | A     | 9   | VAL  | N-CA-CB  | 5.23  | 117.26      | 110.99   |
| 1   | F     | 116 | ASP  | CA-CB-CG | 5.22  | 117.82      | 112.60   |
| 1   | B     | 60  | THR  | CB-CA-C  | 5.22  | 118.78      | 109.65   |
| 1   | J     | 24  | PHE  | CA-CB-CG | 5.22  | 119.02      | 113.80   |
| 1   | F     | 168 | ARG  | N-CA-C   | -5.21 | 105.72      | 111.71   |
| 1   | G     | 137 | ASN  | CA-CB-CG | 5.21  | 117.81      | 112.60   |
| 1   | G     | 175 | ASP  | CA-CB-CG | 5.21  | 117.81      | 112.60   |
| 1   | G     | 24  | PHE  | CA-CB-CG | 5.20  | 119.00      | 113.80   |
| 1   | I     | 24  | PHE  | CA-CB-CG | 5.19  | 118.99      | 113.80   |
| 1   | J     | 229 | LYS  | N-CA-C   | 5.18  | 115.12      | 108.34   |
| 1   | J     | 150 | ASP  | CA-CB-CG | 5.17  | 117.77      | 112.60   |
| 1   | J     | 86  | LEU  | CA-C-N   | 5.16  | 127.45      | 120.38   |
| 1   | J     | 86  | LEU  | C-N-CA   | 5.16  | 127.45      | 120.38   |
| 1   | J     | 60  | THR  | CB-CA-C  | 5.16  | 118.08      | 110.14   |
| 1   | C     | 96  | LYS  | CA-C-N   | 5.15  | 127.50      | 120.54   |
| 1   | C     | 96  | LYS  | C-N-CA   | 5.15  | 127.50      | 120.54   |
| 1   | F     | 96  | LYS  | CA-C-N   | 5.15  | 127.49      | 120.54   |
| 1   | F     | 96  | LYS  | C-N-CA   | 5.15  | 127.49      | 120.54   |
| 1   | C     | 67  | VAL  | CB-CA-C  | -5.15 | 105.19      | 112.14   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 175 | ASP  | CA-CB-CG | 5.13  | 117.73      | 112.60   |
| 1   | I     | 150 | ASP  | CA-CB-CG | 5.13  | 117.73      | 112.60   |
| 1   | D     | 24  | PHE  | CA-CB-CG | 5.12  | 118.92      | 113.80   |
| 1   | D     | 67  | VAL  | CB-CA-C  | -5.12 | 105.23      | 112.14   |
| 1   | F     | 60  | THR  | CB-CA-C  | 5.11  | 118.02      | 110.14   |
| 1   | F     | 37  | GLN  | CA-C-N   | 5.10  | 128.06      | 120.31   |
| 1   | F     | 37  | GLN  | C-N-CA   | 5.10  | 128.06      | 120.31   |
| 1   | F     | 167 | GLU  | CA-C-N   | 5.09  | 127.62      | 120.28   |
| 1   | F     | 167 | GLU  | C-N-CA   | 5.09  | 127.62      | 120.28   |
| 1   | B     | 202 | ASN  | CA-CB-CG | 5.08  | 117.68      | 112.60   |
| 1   | F     | 86  | LEU  | CA-C-N   | 5.08  | 127.08      | 120.28   |
| 1   | F     | 86  | LEU  | C-N-CA   | 5.08  | 127.08      | 120.28   |
| 1   | G     | 42  | ASP  | CA-C-N   | 5.06  | 128.41      | 120.82   |
| 1   | G     | 42  | ASP  | C-N-CA   | 5.06  | 128.41      | 120.82   |
| 1   | F     | 41  | GLU  | CA-C-N   | 5.06  | 131.20      | 121.54   |
| 1   | F     | 41  | GLU  | C-N-CA   | 5.06  | 131.20      | 121.54   |
| 1   | G     | 163 | ASP  | N-CA-C   | -5.06 | 107.39      | 113.21   |
| 1   | I     | 149 | ASP  | CA-CB-CG | 5.05  | 117.65      | 112.60   |
| 1   | H     | 149 | ASP  | CA-CB-CG | 5.05  | 117.65      | 112.60   |
| 1   | F     | 137 | ASN  | CA-CB-CG | 5.04  | 117.64      | 112.60   |
| 1   | C     | 161 | PRO  | CA-C-N   | 5.04  | 127.03      | 120.28   |
| 1   | C     | 161 | PRO  | C-N-CA   | 5.04  | 127.03      | 120.28   |
| 1   | G     | 213 | ILE  | CA-C-N   | 5.04  | 128.43      | 120.97   |
| 1   | G     | 213 | ILE  | C-N-CA   | 5.04  | 128.43      | 120.97   |
| 1   | H     | 137 | ASN  | CA-CB-CG | 5.04  | 117.64      | 112.60   |
| 1   | A     | 24  | PHE  | CA-CB-CG | 5.04  | 118.84      | 113.80   |
| 1   | A     | 116 | ASP  | CA-CB-CG | 5.02  | 117.62      | 112.60   |
| 1   | A     | 201 | ARG  | N-CA-C   | -5.02 | 101.53      | 109.96   |
| 1   | H     | 90  | GLU  | CB-CG-CD | 5.02  | 121.13      | 112.60   |
| 1   | D     | 86  | LEU  | CA-C-N   | 5.01  | 127.00      | 120.28   |
| 1   | D     | 86  | LEU  | C-N-CA   | 5.01  | 127.00      | 120.28   |
| 1   | I     | 60  | THR  | CB-CA-C  | 5.01  | 117.86      | 110.14   |
| 1   | E     | 42  | ASP  | CA-C-N   | 5.01  | 128.33      | 120.82   |
| 1   | E     | 42  | ASP  | C-N-CA   | 5.01  | 128.33      | 120.82   |
| 1   | H     | 67  | VAL  | CB-CA-C  | -5.01 | 105.48      | 112.04   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1893  | 0        | 1848     | 25      | 0            |
| 1   | B     | 1893  | 0        | 1848     | 20      | 0            |
| 1   | C     | 1892  | 0        | 1849     | 20      | 0            |
| 1   | D     | 1885  | 0        | 1842     | 17      | 0            |
| 1   | E     | 1880  | 0        | 1835     | 21      | 0            |
| 1   | F     | 1842  | 0        | 1801     | 25      | 0            |
| 1   | G     | 1846  | 0        | 1801     | 24      | 0            |
| 1   | H     | 1886  | 0        | 1841     | 22      | 0            |
| 1   | I     | 1874  | 0        | 1829     | 18      | 0            |
| 1   | J     | 1874  | 0        | 1829     | 19      | 0            |
| 2   | A     | 15    | 0        | 0        | 0       | 0            |
| 2   | B     | 8     | 0        | 0        | 0       | 0            |
| 2   | C     | 5     | 0        | 0        | 0       | 0            |
| 2   | D     | 9     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 1       | 0            |
| 2   | H     | 4     | 0        | 0        | 0       | 0            |
| 2   | I     | 5     | 0        | 0        | 0       | 0            |
| 2   | J     | 7     | 0        | 0        | 0       | 0            |
| All | All   | 18821 | 0        | 18323    | 208     | 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 6.

All (208) 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:C:222:ARG:HH21 | 1:C:222:ARG:HG3 | 1.24                     | 1.03              |
| 1:D:222:ARG:HH21 | 1:D:222:ARG:HG3 | 1.24                     | 1.02              |
| 1:G:222:ARG:HH21 | 1:G:222:ARG:HG3 | 1.26                     | 1.01              |
| 1:J:222:ARG:HH21 | 1:J:222:ARG:HG3 | 1.25                     | 1.01              |
| 1:F:222:ARG:HH21 | 1:F:222:ARG:HG3 | 1.26                     | 1.00              |
| 1:A:222:ARG:HH21 | 1:A:222:ARG:HG3 | 1.28                     | 0.99              |
| 1:B:222:ARG:HH21 | 1:B:222:ARG:HG3 | 1.27                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:222:ARG:HH21 | 1:I:222:ARG:HG3  | 1.26                     | 0.96              |
| 1:H:222:ARG:HH21 | 1:H:222:ARG:HG3  | 1.27                     | 0.94              |
| 1:J:9:VAL:HG11   | 1:J:43:GLU:HB3   | 1.54                     | 0.89              |
| 1:H:184:MET:HE1  | 1:H:208:THR:HB   | 1.63                     | 0.80              |
| 1:I:8:ILE:HD12   | 1:I:231:TYR:HB2  | 1.64                     | 0.78              |
| 1:D:133:GLU:HG3  | 1:D:212:LEU:HD21 | 1.68                     | 0.75              |
| 1:F:184:MET:HE1  | 1:F:208:THR:HB   | 1.68                     | 0.75              |
| 1:H:133:GLU:HG3  | 1:H:212:LEU:HD21 | 1.69                     | 0.74              |
| 1:B:133:GLU:HG3  | 1:B:212:LEU:HD21 | 1.70                     | 0.74              |
| 1:E:133:GLU:HG3  | 1:E:212:LEU:HD21 | 1.70                     | 0.74              |
| 1:I:133:GLU:HG3  | 1:I:212:LEU:HD21 | 1.69                     | 0.73              |
| 1:E:109:PHE:HE1  | 1:E:111:ILE:HD11 | 1.54                     | 0.72              |
| 1:J:133:GLU:HG3  | 1:J:212:LEU:HD21 | 1.70                     | 0.72              |
| 1:G:133:GLU:HG3  | 1:G:212:LEU:HD21 | 1.71                     | 0.72              |
| 1:A:133:GLU:HG3  | 1:A:212:LEU:HD21 | 1.69                     | 0.72              |
| 1:F:133:GLU:HG3  | 1:F:212:LEU:HD21 | 1.71                     | 0.72              |
| 1:C:184:MET:HE1  | 1:C:208:THR:HB   | 1.73                     | 0.70              |
| 1:G:184:MET:HE1  | 1:G:208:THR:HB   | 1.74                     | 0.69              |
| 1:A:184:MET:CE   | 1:A:208:THR:HB   | 2.23                     | 0.69              |
| 1:J:14:ARG:HG2   | 1:J:15:GLU:HG2   | 1.78                     | 0.66              |
| 1:H:222:ARG:HG3  | 1:H:222:ARG:NH2  | 2.07                     | 0.63              |
| 1:J:9:VAL:CG1    | 1:J:43:GLU:HB3   | 2.29                     | 0.62              |
| 1:F:22:LYS:HG3   | 1:F:23:LEU:HD13  | 1.81                     | 0.61              |
| 1:B:222:ARG:HG3  | 1:B:222:ARG:NH2  | 2.06                     | 0.61              |
| 1:G:217:HIS:HB2  | 2:G:301:HOH:O    | 2.01                     | 0.61              |
| 1:C:60:THR:HB    | 1:C:110:GLU:HB3  | 1.84                     | 0.59              |
| 1:C:222:ARG:HG3  | 1:C:222:ARG:NH2  | 2.03                     | 0.59              |
| 1:C:133:GLU:HG3  | 1:C:212:LEU:HD21 | 1.85                     | 0.59              |
| 1:I:222:ARG:HG3  | 1:I:222:ARG:NH2  | 2.06                     | 0.59              |
| 1:F:60:THR:HB    | 1:F:110:GLU:HB3  | 1.85                     | 0.58              |
| 1:B:10:LYS:HB2   | 1:B:231:TYR:HE2  | 1.68                     | 0.58              |
| 1:A:196:VAL:HG22 | 1:A:224:VAL:HB   | 1.86                     | 0.58              |
| 1:J:60:THR:HB    | 1:J:110:GLU:HB3  | 1.85                     | 0.58              |
| 1:H:184:MET:CE   | 1:H:208:THR:HB   | 2.34                     | 0.58              |
| 1:F:222:ARG:HG3  | 1:F:222:ARG:NH2  | 2.05                     | 0.57              |
| 1:I:60:THR:HB    | 1:I:110:GLU:HB3  | 1.85                     | 0.57              |
| 1:F:184:MET:CE   | 1:F:208:THR:HB   | 2.34                     | 0.57              |
| 1:D:222:ARG:HG3  | 1:D:222:ARG:NH2  | 2.03                     | 0.57              |
| 1:G:162:ALA:C    | 1:G:164:VAL:H    | 2.12                     | 0.57              |
| 1:H:60:THR:HB    | 1:H:110:GLU:HB3  | 1.86                     | 0.56              |
| 1:J:85:GLN:O     | 1:J:89:LYS:HG2   | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:60:THR:HB    | 1:A:110:GLU:HB3  | 1.86                     | 0.56              |
| 1:D:75:MET:HA    | 1:D:75:MET:HE2   | 1.88                     | 0.56              |
| 1:E:183:VAL:O    | 1:E:186:LEU:HB2  | 2.05                     | 0.56              |
| 1:B:197:TYR:HE2  | 1:B:199:SER:HG   | 1.53                     | 0.56              |
| 1:B:60:THR:HB    | 1:B:110:GLU:HB3  | 1.87                     | 0.55              |
| 1:F:168:ARG:HG3  | 1:F:171:ARG:HH22 | 1.72                     | 0.55              |
| 1:A:18:VAL:O     | 1:A:22:LYS:HG3   | 2.06                     | 0.54              |
| 1:E:109:PHE:CE1  | 1:E:111:ILE:HD11 | 2.38                     | 0.54              |
| 1:A:9:VAL:HG21   | 1:A:43:GLU:HB3   | 1.90                     | 0.54              |
| 1:J:124:ILE:HD12 | 1:J:124:ILE:H    | 1.73                     | 0.54              |
| 1:B:8:ILE:HD11   | 1:B:10:LYS:HE2   | 1.90                     | 0.54              |
| 1:C:59:CYS:O     | 1:C:109:PHE:HA   | 2.09                     | 0.53              |
| 1:G:60:THR:HB    | 1:G:110:GLU:HB3  | 1.91                     | 0.53              |
| 1:B:75:MET:HA    | 1:B:75:MET:HE2   | 1.91                     | 0.53              |
| 1:E:7:ARG:HB2    | 1:E:230:LYS:HD2  | 1.89                     | 0.53              |
| 1:H:79:THR:OG1   | 1:H:82:GLU:HG3   | 2.10                     | 0.52              |
| 1:J:222:ARG:HG3  | 1:J:222:ARG:NH2  | 2.05                     | 0.52              |
| 1:G:222:ARG:HG3  | 1:G:222:ARG:NH2  | 2.05                     | 0.52              |
| 1:H:75:MET:HE2   | 1:H:75:MET:HA    | 1.91                     | 0.52              |
| 1:F:155:TYR:HB3  | 1:F:156:LEU:HD22 | 1.91                     | 0.52              |
| 1:A:75:MET:HE2   | 1:A:75:MET:HA    | 1.90                     | 0.52              |
| 1:A:59:CYS:O     | 1:A:109:PHE:HA   | 2.10                     | 0.52              |
| 1:F:227:ARG:HG3  | 1:F:227:ARG:HH11 | 1.75                     | 0.52              |
| 1:C:75:MET:HE2   | 1:C:75:MET:HA    | 1.92                     | 0.51              |
| 1:G:59:CYS:O     | 1:G:109:PHE:HA   | 2.10                     | 0.51              |
| 1:G:184:MET:CE   | 1:G:208:THR:HB   | 2.38                     | 0.51              |
| 1:A:184:MET:HE1  | 1:A:208:THR:HB   | 1.91                     | 0.51              |
| 1:C:184:MET:CE   | 1:C:208:THR:HB   | 2.39                     | 0.51              |
| 1:F:59:CYS:O     | 1:F:109:PHE:HA   | 2.10                     | 0.51              |
| 1:B:59:CYS:O     | 1:B:109:PHE:HA   | 2.10                     | 0.51              |
| 1:B:10:LYS:HB2   | 1:B:231:TYR:CE2  | 2.46                     | 0.51              |
| 1:I:59:CYS:O     | 1:I:109:PHE:HA   | 2.11                     | 0.51              |
| 1:A:184:MET:HG3  | 1:A:205:MET:HE3  | 1.93                     | 0.50              |
| 1:H:59:CYS:O     | 1:H:109:PHE:HA   | 2.11                     | 0.50              |
| 1:G:184:MET:HE2  | 1:G:205:MET:HG2  | 1.93                     | 0.50              |
| 1:A:145:HIS:HA   | 1:A:148:ILE:HD12 | 1.94                     | 0.50              |
| 1:A:222:ARG:HG3  | 1:A:222:ARG:NH2  | 2.07                     | 0.50              |
| 1:D:22:LYS:HG3   | 1:D:23:LEU:HD13  | 1.93                     | 0.49              |
| 1:J:59:CYS:O     | 1:J:109:PHE:HA   | 2.12                     | 0.49              |
| 1:F:75:MET:HE2   | 1:F:75:MET:HA    | 1.94                     | 0.49              |
| 1:G:184:MET:HE1  | 1:G:205:MET:HA   | 1.94                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:79:THR:HG22 | 1:B:81:GLU:H     | 1.78                     | 0.49              |
| 1:E:75:MET:HE2  | 1:E:75:MET:HA    | 1.93                     | 0.48              |
| 1:F:168:ARG:HG3 | 1:F:171:ARG:NH2  | 2.28                     | 0.48              |
| 1:B:7:ARG:HG2   | 1:B:7:ARG:HH11   | 1.78                     | 0.48              |
| 1:C:14:ARG:HD2  | 1:C:15:GLU:HG2   | 1.95                     | 0.48              |
| 1:A:9:VAL:CG2   | 1:A:43:GLU:HB3   | 2.44                     | 0.47              |
| 1:B:33:ILE:O    | 1:B:64:ASP:HB2   | 2.13                     | 0.47              |
| 1:E:21:ARG:CZ   | 1:H:124:ILE:HD11 | 2.44                     | 0.47              |
| 1:I:44:LYS:O    | 1:I:48:VAL:HG23  | 2.14                     | 0.47              |
| 1:D:59:CYS:O    | 1:D:109:PHE:HA   | 2.14                     | 0.47              |
| 1:D:194:PHE:CD1 | 1:D:222:ARG:HB2  | 2.50                     | 0.47              |
| 1:H:9:VAL:HG13  | 1:H:43:GLU:HB3   | 1.97                     | 0.47              |
| 1:C:194:PHE:CD1 | 1:C:222:ARG:HB2  | 2.50                     | 0.47              |
| 1:G:194:PHE:CD1 | 1:G:222:ARG:HB2  | 2.50                     | 0.47              |
| 1:J:194:PHE:CD1 | 1:J:222:ARG:HB2  | 2.49                     | 0.47              |
| 1:J:22:LYS:HG3  | 1:J:23:LEU:HD13  | 1.96                     | 0.47              |
| 1:J:117:TRP:HB3 | 1:J:183:VAL:HG13 | 1.97                     | 0.47              |
| 1:G:174:LEU:O   | 1:G:178:ILE:HG12 | 2.16                     | 0.46              |
| 1:H:194:PHE:CD1 | 1:H:222:ARG:HB2  | 2.51                     | 0.46              |
| 1:C:184:MET:HE2 | 1:C:205:MET:HG2  | 1.98                     | 0.46              |
| 1:H:184:MET:HE2 | 1:H:205:MET:HG2  | 1.98                     | 0.46              |
| 1:I:194:PHE:CD1 | 1:I:222:ARG:HB2  | 2.51                     | 0.46              |
| 1:C:9:VAL:HG22  | 1:C:230:LYS:HG3  | 1.97                     | 0.46              |
| 1:C:22:LYS:HG3  | 1:C:23:LEU:HD13  | 1.98                     | 0.45              |
| 1:C:97:ARG:O    | 1:C:100:ARG:HD3  | 2.17                     | 0.45              |
| 1:F:187:TRP:HB2 | 1:F:221:LEU:HD21 | 1.98                     | 0.45              |
| 1:F:44:LYS:O    | 1:F:48:VAL:HG23  | 2.17                     | 0.45              |
| 1:F:194:PHE:CD1 | 1:F:222:ARG:HB2  | 2.51                     | 0.45              |
| 1:I:117:TRP:HB3 | 1:I:183:VAL:HG13 | 1.99                     | 0.45              |
| 1:A:117:TRP:HB3 | 1:A:183:VAL:HG13 | 1.99                     | 0.45              |
| 1:C:184:MET:HE1 | 1:C:205:MET:HA   | 1.98                     | 0.45              |
| 1:E:60:THR:HB   | 1:E:110:GLU:HB3  | 1.97                     | 0.45              |
| 1:G:46:ALA:HB2  | 1:G:101:PHE:CD1  | 2.52                     | 0.45              |
| 1:C:93:GLU:HA   | 1:C:96:LYS:HE3   | 1.99                     | 0.44              |
| 1:E:194:PHE:CD1 | 1:E:222:ARG:HB2  | 2.52                     | 0.44              |
| 1:H:22:LYS:O    | 1:H:25:PRO:HD2   | 2.18                     | 0.44              |
| 1:G:117:TRP:HB3 | 1:G:183:VAL:HG13 | 1.99                     | 0.44              |
| 1:A:194:PHE:CD1 | 1:A:222:ARG:HB2  | 2.52                     | 0.44              |
| 1:J:75:MET:HE2  | 1:J:75:MET:HA    | 1.99                     | 0.44              |
| 1:E:187:TRP:HB2 | 1:E:221:LEU:HD21 | 2.00                     | 0.44              |
| 1:A:184:MET:CG  | 1:A:205:MET:HE3  | 2.48                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:184:MET:HE2 | 1:F:205:MET:HG2  | 2.00                     | 0.44              |
| 1:F:141:GLN:HG2 | 1:F:145:HIS:CE1  | 2.53                     | 0.43              |
| 1:D:141:GLN:HG2 | 1:D:145:HIS:CE1  | 2.54                     | 0.43              |
| 1:F:184:MET:HE1 | 1:F:205:MET:HA   | 1.99                     | 0.43              |
| 1:H:93:GLU:HA   | 1:H:96:LYS:HE3   | 2.00                     | 0.43              |
| 1:H:141:GLN:HG2 | 1:H:145:HIS:CE1  | 2.53                     | 0.43              |
| 1:I:93:GLU:HA   | 1:I:96:LYS:HE3   | 1.99                     | 0.43              |
| 1:E:79:THR:HB   | 1:E:82:GLU:HG3   | 2.00                     | 0.43              |
| 1:F:93:GLU:O    | 1:F:96:LYS:HB2   | 2.19                     | 0.43              |
| 1:G:9:VAL:HG22  | 1:G:230:LYS:HG3  | 1.99                     | 0.43              |
| 1:G:141:GLN:HG2 | 1:G:145:HIS:CE1  | 2.53                     | 0.43              |
| 1:F:97:ARG:O    | 1:F:100:ARG:HD3  | 2.18                     | 0.43              |
| 1:J:97:ARG:O    | 1:J:100:ARG:HD3  | 2.18                     | 0.43              |
| 1:D:97:ARG:O    | 1:D:100:ARG:HD3  | 2.18                     | 0.43              |
| 1:I:195:GLU:CD  | 1:I:201:ARG:NH2  | 2.77                     | 0.43              |
| 1:G:97:ARG:O    | 1:G:100:ARG:HD3  | 2.19                     | 0.43              |
| 1:B:18:VAL:O    | 1:B:22:LYS:HG3   | 2.18                     | 0.43              |
| 1:E:8:ILE:HG23  | 1:E:231:TYR:HD2  | 1.82                     | 0.43              |
| 1:E:141:GLN:HG2 | 1:E:145:HIS:CE1  | 2.53                     | 0.43              |
| 1:I:187:TRP:HB2 | 1:I:221:LEU:HD21 | 2.01                     | 0.42              |
| 1:I:195:GLU:OE2 | 1:I:201:ARG:NH2  | 2.53                     | 0.42              |
| 1:J:187:TRP:HB2 | 1:J:221:LEU:HD21 | 2.01                     | 0.42              |
| 1:D:75:MET:HE1  | 1:D:164:VAL:HA   | 2.00                     | 0.42              |
| 1:E:79:THR:HG22 | 1:E:81:GLU:H     | 1.84                     | 0.42              |
| 1:G:8:ILE:HD11  | 1:G:43:GLU:OE2   | 2.18                     | 0.42              |
| 1:A:13:PHE:CE1  | 1:A:51:LEU:HD11  | 2.55                     | 0.42              |
| 1:D:165:ASP:CG  | 1:D:168:ARG:HB2  | 2.44                     | 0.42              |
| 1:E:67:VAL:HG22 | 1:E:114:TRP:CD2  | 2.55                     | 0.42              |
| 1:F:84:TYR:O    | 1:F:88:VAL:HG23  | 2.19                     | 0.42              |
| 1:H:44:LYS:O    | 1:H:48:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:97:ARG:O    | 1:A:100:ARG:HD3  | 2.20                     | 0.42              |
| 1:B:194:PHE:CD1 | 1:B:222:ARG:HB2  | 2.54                     | 0.42              |
| 1:D:44:LYS:O    | 1:D:48:VAL:HG23  | 2.19                     | 0.42              |
| 1:D:187:TRP:HB2 | 1:D:221:LEU:HD21 | 2.02                     | 0.42              |
| 1:I:75:MET:HE2  | 1:I:159:PHE:CD2  | 2.55                     | 0.42              |
| 1:A:187:TRP:HB2 | 1:A:221:LEU:HD21 | 2.02                     | 0.42              |
| 1:G:187:TRP:HB2 | 1:G:221:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:31:MET:HE3  | 1:A:61:ILE:HG12  | 2.01                     | 0.42              |
| 1:B:117:TRP:HB3 | 1:B:183:VAL:HG13 | 2.01                     | 0.42              |
| 1:C:141:GLN:HG2 | 1:C:145:HIS:CE1  | 2.54                     | 0.41              |
| 1:I:160:SER:HB3 | 1:I:163:ASP:OD2  | 2.20                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:141:GLN:HG2 | 1:J:145:HIS:CE1  | 2.55                     | 0.41              |
| 1:C:117:TRP:HB3 | 1:C:183:VAL:HG13 | 2.02                     | 0.41              |
| 1:D:70:HIS:HB2  | 1:D:176:TYR:HB2  | 2.01                     | 0.41              |
| 1:D:93:GLU:HA   | 1:D:96:LYS:HE3   | 2.01                     | 0.41              |
| 1:B:44:LYS:O    | 1:B:48:VAL:HG23  | 2.19                     | 0.41              |
| 1:B:187:TRP:HB2 | 1:B:221:LEU:HD21 | 2.01                     | 0.41              |
| 1:D:9:VAL:HG22  | 1:D:230:LYS:HG3  | 2.02                     | 0.41              |
| 1:F:39:ILE:HG22 | 1:F:228:PHE:HE2  | 1.85                     | 0.41              |
| 1:H:187:TRP:HB2 | 1:H:221:LEU:HD21 | 2.02                     | 0.41              |
| 1:C:187:TRP:HB2 | 1:C:221:LEU:HD21 | 2.02                     | 0.41              |
| 1:I:97:ARG:O    | 1:I:100:ARG:HD3  | 2.20                     | 0.41              |
| 1:A:141:GLN:HG2 | 1:A:145:HIS:CE1  | 2.55                     | 0.41              |
| 1:F:79:THR:HG22 | 1:F:81:GLU:H     | 1.86                     | 0.41              |
| 1:F:117:TRP:HB3 | 1:F:183:VAL:HG13 | 2.02                     | 0.41              |
| 1:G:93:GLU:HA   | 1:G:96:LYS:HE3   | 2.02                     | 0.41              |
| 1:A:184:MET:HE2 | 1:A:205:MET:HA   | 2.03                     | 0.41              |
| 1:C:99:GLN:HA   | 1:C:102:TYR:CE1  | 2.55                     | 0.41              |
| 1:I:141:GLN:HG2 | 1:I:145:HIS:CE1  | 2.55                     | 0.41              |
| 1:E:30:LEU:O    | 1:E:32:PRO:HD3   | 2.20                     | 0.41              |
| 1:G:217:HIS:HA  | 1:G:218:PRO:HD3  | 1.84                     | 0.41              |
| 1:H:117:TRP:HB3 | 1:H:183:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:93:GLU:HA   | 1:A:96:LYS:HE3   | 2.01                     | 0.41              |
| 1:B:31:MET:HE3  | 1:B:61:ILE:HG12  | 2.02                     | 0.41              |
| 1:B:93:GLU:HA   | 1:B:96:LYS:HE3   | 2.03                     | 0.41              |
| 1:D:117:TRP:HB3 | 1:D:183:VAL:HG13 | 2.03                     | 0.41              |
| 1:E:97:ARG:O    | 1:E:100:ARG:HD3  | 2.20                     | 0.41              |
| 1:E:84:TYR:O    | 1:E:88:VAL:HG23  | 2.21                     | 0.40              |
| 1:H:184:MET:HE1 | 1:H:205:MET:HA   | 2.03                     | 0.40              |
| 1:A:21:ARG:NH1  | 1:E:118:TYR:CZ   | 2.89                     | 0.40              |
| 1:J:40:HIS:C    | 1:J:45:PHE:HB2   | 2.46                     | 0.40              |
| 1:J:67:VAL:HG22 | 1:J:114:TRP:CD2  | 2.57                     | 0.40              |
| 1:E:52:ILE:HD11 | 1:E:196:VAL:HG11 | 2.02                     | 0.40              |
| 1:G:44:LYS:O    | 1:G:48:VAL:HG23  | 2.20                     | 0.40              |
| 1:G:44:LYS:O    | 1:G:47:ALA:HB3   | 2.21                     | 0.40              |
| 1:H:45:PHE:CZ   | 1:H:49:ILE:HD11  | 2.56                     | 0.40              |
| 1:E:18:VAL:HG11 | 1:H:127:HIS:CD2  | 2.57                     | 0.40              |
| 1:I:43:GLU:H    | 1:I:43:GLU:HG2   | 1.61                     | 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     | 224/266 (84%)   | 216 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 1   | B     | 224/266 (84%)   | 218 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 1   | C     | 224/266 (84%)   | 216 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 1   | D     | 223/266 (84%)   | 216 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 1   | E     | 220/266 (83%)   | 210 (96%)  | 9 (4%)  | 1 (0%)   | 24          | 52  |
| 1   | F     | 216/266 (81%)   | 208 (96%)  | 7 (3%)  | 1 (0%)   | 24          | 52  |
| 1   | G     | 217/266 (82%)   | 205 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 1   | H     | 224/266 (84%)   | 215 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 1   | I     | 222/266 (84%)   | 214 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 1   | J     | 222/266 (84%)   | 215 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| All | All   | 2216/2660 (83%) | 2133 (96%) | 81 (4%) | 2 (0%)   | 48          | 75  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 42  | ASP  |
| 1   | E     | 42  | ASP  |

### 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     | 206/240 (86%) | 183 (89%) | 23 (11%) | 6           | 20 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | B     | 206/240 (86%)   | 183 (89%)  | 23 (11%)  | 6           | 20 |
| 1   | C     | 206/240 (86%)   | 187 (91%)  | 19 (9%)   | 8           | 28 |
| 1   | D     | 205/240 (85%)   | 188 (92%)  | 17 (8%)   | 10          | 32 |
| 1   | E     | 204/240 (85%)   | 185 (91%)  | 19 (9%)   | 8           | 28 |
| 1   | F     | 201/240 (84%)   | 178 (89%)  | 23 (11%)  | 5           | 20 |
| 1   | G     | 201/240 (84%)   | 184 (92%)  | 17 (8%)   | 10          | 31 |
| 1   | H     | 205/240 (85%)   | 186 (91%)  | 19 (9%)   | 8           | 28 |
| 1   | I     | 204/240 (85%)   | 187 (92%)  | 17 (8%)   | 10          | 32 |
| 1   | J     | 204/240 (85%)   | 187 (92%)  | 17 (8%)   | 10          | 32 |
| All | All   | 2042/2400 (85%) | 1848 (90%) | 194 (10%) | 8           | 27 |

All (194) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | ILE  |
| 1   | A     | 9   | VAL  |
| 1   | A     | 10  | LYS  |
| 1   | A     | 14  | ARG  |
| 1   | A     | 23  | LEU  |
| 1   | A     | 34  | SER  |
| 1   | A     | 60  | THR  |
| 1   | A     | 66  | SER  |
| 1   | A     | 67  | VAL  |
| 1   | A     | 68  | GLN  |
| 1   | A     | 99  | GLN  |
| 1   | A     | 113 | ARG  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 154 | ARG  |
| 1   | A     | 158 | ARG  |
| 1   | A     | 160 | SER  |
| 1   | A     | 163 | ASP  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 184 | MET  |
| 1   | A     | 186 | LEU  |
| 1   | A     | 214 | LYS  |
| 1   | A     | 221 | LEU  |
| 1   | A     | 222 | ARG  |
| 1   | B     | 8   | ILE  |
| 1   | B     | 14  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 18  | VAL  |
| 1   | B     | 23  | LEU  |
| 1   | B     | 39  | ILE  |
| 1   | B     | 51  | LEU  |
| 1   | B     | 60  | THR  |
| 1   | B     | 62  | LEU  |
| 1   | B     | 67  | VAL  |
| 1   | B     | 99  | GLN  |
| 1   | B     | 113 | ARG  |
| 1   | B     | 131 | GLN  |
| 1   | B     | 147 | ASN  |
| 1   | B     | 158 | ARG  |
| 1   | B     | 163 | ASP  |
| 1   | B     | 174 | LEU  |
| 1   | B     | 186 | LEU  |
| 1   | B     | 199 | SER  |
| 1   | B     | 214 | LYS  |
| 1   | B     | 221 | LEU  |
| 1   | B     | 222 | ARG  |
| 1   | B     | 227 | ARG  |
| 1   | B     | 229 | LYS  |
| 1   | C     | 7   | ARG  |
| 1   | C     | 14  | ARG  |
| 1   | C     | 23  | LEU  |
| 1   | C     | 60  | THR  |
| 1   | C     | 62  | LEU  |
| 1   | C     | 67  | VAL  |
| 1   | C     | 99  | GLN  |
| 1   | C     | 113 | ARG  |
| 1   | C     | 131 | GLN  |
| 1   | C     | 147 | ASN  |
| 1   | C     | 149 | ASP  |
| 1   | C     | 158 | ARG  |
| 1   | C     | 163 | ASP  |
| 1   | C     | 174 | LEU  |
| 1   | C     | 184 | MET  |
| 1   | C     | 186 | LEU  |
| 1   | C     | 199 | SER  |
| 1   | C     | 221 | LEU  |
| 1   | C     | 222 | ARG  |
| 1   | D     | 7   | ARG  |
| 1   | D     | 15  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 23  | LEU  |
| 1   | D     | 43  | GLU  |
| 1   | D     | 62  | LEU  |
| 1   | D     | 67  | VAL  |
| 1   | D     | 99  | GLN  |
| 1   | D     | 113 | ARG  |
| 1   | D     | 147 | ASN  |
| 1   | D     | 158 | ARG  |
| 1   | D     | 160 | SER  |
| 1   | D     | 163 | ASP  |
| 1   | D     | 167 | GLU  |
| 1   | D     | 174 | LEU  |
| 1   | D     | 199 | SER  |
| 1   | D     | 221 | LEU  |
| 1   | D     | 222 | ARG  |
| 1   | E     | 6   | ASN  |
| 1   | E     | 7   | ARG  |
| 1   | E     | 15  | GLU  |
| 1   | E     | 41  | GLU  |
| 1   | E     | 60  | THR  |
| 1   | E     | 67  | VAL  |
| 1   | E     | 99  | GLN  |
| 1   | E     | 113 | ARG  |
| 1   | E     | 147 | ASN  |
| 1   | E     | 149 | ASP  |
| 1   | E     | 154 | ARG  |
| 1   | E     | 158 | ARG  |
| 1   | E     | 159 | PHE  |
| 1   | E     | 174 | LEU  |
| 1   | E     | 199 | SER  |
| 1   | E     | 210 | GLU  |
| 1   | E     | 221 | LEU  |
| 1   | E     | 229 | LYS  |
| 1   | E     | 230 | LYS  |
| 1   | F     | 15  | GLU  |
| 1   | F     | 20  | GLU  |
| 1   | F     | 23  | LEU  |
| 1   | F     | 39  | ILE  |
| 1   | F     | 60  | THR  |
| 1   | F     | 62  | LEU  |
| 1   | F     | 67  | VAL  |
| 1   | F     | 97  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 99  | GLN  |
| 1   | F     | 113 | ARG  |
| 1   | F     | 132 | LYS  |
| 1   | F     | 147 | ASN  |
| 1   | F     | 150 | ASP  |
| 1   | F     | 156 | LEU  |
| 1   | F     | 158 | ARG  |
| 1   | F     | 174 | LEU  |
| 1   | F     | 184 | MET  |
| 1   | F     | 186 | LEU  |
| 1   | F     | 199 | SER  |
| 1   | F     | 221 | LEU  |
| 1   | F     | 222 | ARG  |
| 1   | F     | 229 | LYS  |
| 1   | F     | 230 | LYS  |
| 1   | G     | 8   | ILE  |
| 1   | G     | 9   | VAL  |
| 1   | G     | 60  | THR  |
| 1   | G     | 62  | LEU  |
| 1   | G     | 67  | VAL  |
| 1   | G     | 90  | GLU  |
| 1   | G     | 113 | ARG  |
| 1   | G     | 131 | GLN  |
| 1   | G     | 147 | ASN  |
| 1   | G     | 156 | LEU  |
| 1   | G     | 163 | ASP  |
| 1   | G     | 174 | LEU  |
| 1   | G     | 184 | MET  |
| 1   | G     | 186 | LEU  |
| 1   | G     | 199 | SER  |
| 1   | G     | 221 | LEU  |
| 1   | G     | 222 | ARG  |
| 1   | H     | 8   | ILE  |
| 1   | H     | 9   | VAL  |
| 1   | H     | 35  | VAL  |
| 1   | H     | 49  | ILE  |
| 1   | H     | 60  | THR  |
| 1   | H     | 62  | LEU  |
| 1   | H     | 67  | VAL  |
| 1   | H     | 90  | GLU  |
| 1   | H     | 99  | GLN  |
| 1   | H     | 113 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 147 | ASN  |
| 1   | H     | 154 | ARG  |
| 1   | H     | 158 | ARG  |
| 1   | H     | 163 | ASP  |
| 1   | H     | 174 | LEU  |
| 1   | H     | 184 | MET  |
| 1   | H     | 199 | SER  |
| 1   | H     | 221 | LEU  |
| 1   | H     | 222 | ARG  |
| 1   | I     | 8   | ILE  |
| 1   | I     | 23  | LEU  |
| 1   | I     | 43  | GLU  |
| 1   | I     | 60  | THR  |
| 1   | I     | 62  | LEU  |
| 1   | I     | 67  | VAL  |
| 1   | I     | 99  | GLN  |
| 1   | I     | 113 | ARG  |
| 1   | I     | 147 | ASN  |
| 1   | I     | 158 | ARG  |
| 1   | I     | 163 | ASP  |
| 1   | I     | 174 | LEU  |
| 1   | I     | 186 | LEU  |
| 1   | I     | 199 | SER  |
| 1   | I     | 201 | ARG  |
| 1   | I     | 221 | LEU  |
| 1   | I     | 222 | ARG  |
| 1   | J     | 8   | ILE  |
| 1   | J     | 14  | ARG  |
| 1   | J     | 15  | GLU  |
| 1   | J     | 23  | LEU  |
| 1   | J     | 60  | THR  |
| 1   | J     | 62  | LEU  |
| 1   | J     | 67  | VAL  |
| 1   | J     | 99  | GLN  |
| 1   | J     | 113 | ARG  |
| 1   | J     | 126 | SER  |
| 1   | J     | 160 | SER  |
| 1   | J     | 163 | ASP  |
| 1   | J     | 174 | LEU  |
| 1   | J     | 199 | SER  |
| 1   | J     | 221 | LEU  |
| 1   | J     | 222 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 229 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | GLN  |
| 1   | A     | 98  | ASN  |
| 1   | A     | 104 | GLN  |
| 1   | B     | 16  | ASN  |
| 1   | B     | 98  | ASN  |
| 1   | B     | 104 | GLN  |
| 1   | C     | 26  | GLN  |
| 1   | D     | 26  | GLN  |
| 1   | D     | 104 | GLN  |
| 1   | D     | 131 | GLN  |
| 1   | E     | 104 | GLN  |
| 1   | F     | 26  | GLN  |
| 1   | F     | 125 | ASN  |
| 1   | F     | 131 | GLN  |
| 1   | G     | 26  | GLN  |
| 1   | G     | 104 | GLN  |
| 1   | G     | 131 | GLN  |
| 1   | H     | 26  | GLN  |
| 1   | H     | 68  | GLN  |
| 1   | H     | 104 | GLN  |
| 1   | H     | 131 | GLN  |
| 1   | I     | 26  | GLN  |
| 1   | I     | 104 | GLN  |
| 1   | I     | 131 | GLN  |
| 1   | J     | 26  | GLN  |
| 1   | J     | 40  | HIS  |
| 1   | J     | 104 | GLN  |

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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     | 226/266 (84%)   | -0.16  | 1 (0%) 88 75  | 52, 70, 98, 126       | 0     |
| 1   | B     | 226/266 (84%)   | -0.16  | 0 100 100     | 49, 69, 102, 135      | 0     |
| 1   | C     | 226/266 (84%)   | 0.08   | 1 (0%) 88 75  | 64, 91, 126, 153      | 0     |
| 1   | D     | 225/266 (84%)   | 0.02   | 1 (0%) 88 75  | 60, 89, 120, 149      | 0     |
| 1   | E     | 224/266 (84%)   | 0.08   | 0 100 100     | 65, 95, 130, 160      | 0     |
| 1   | F     | 220/266 (82%)   | 0.34   | 6 (2%) 56 33  | 66, 103, 144, 173     | 0     |
| 1   | G     | 221/266 (83%)   | 0.25   | 1 (0%) 87 72  | 70, 103, 144, 164     | 0     |
| 1   | H     | 226/266 (84%)   | 0.10   | 3 (1%) 75 53  | 73, 97, 122, 139      | 0     |
| 1   | I     | 224/266 (84%)   | 0.11   | 0 100 100     | 76, 100, 123, 129     | 0     |
| 1   | J     | 224/266 (84%)   | 0.15   | 3 (1%) 75 53  | 60, 98, 139, 150      | 0     |
| All | All   | 2242/2660 (84%) | 0.08   | 16 (0%) 84 66 | 49, 93, 130, 173      | 0     |

All (16) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 231 | TYR  | 3.2  |
| 1   | G     | 231 | TYR  | 3.0  |
| 1   | F     | 64  | ASP  | 2.9  |
| 1   | F     | 8   | ILE  | 2.5  |
| 1   | F     | 161 | PRO  | 2.5  |
| 1   | F     | 35  | VAL  | 2.5  |
| 1   | H     | 233 | ALA  | 2.5  |
| 1   | C     | 15  | GLU  | 2.4  |
| 1   | A     | 231 | TYR  | 2.4  |
| 1   | F     | 230 | LYS  | 2.4  |
| 1   | F     | 124 | ILE  | 2.3  |
| 1   | J     | 159 | PHE  | 2.3  |
| 1   | J     | 231 | TYR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 19  | GLU  | 2.1  |
| 1   | H     | 18  | VAL  | 2.1  |
| 1   | J     | 75  | MET  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.