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

Jun 25, 2024 – 01:58 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 6QZ2 |
| Title | : | Structure of MHETase from Ideonella sakaiensis |
| Authors | : | Allen, M.D.; Johnson, C.W.; Knott, B.C.; Beckham, G.T.; McGeehan, J.E. |
| Deposited on | : | 2019-03-10 |
| Resolution | : | 1.90 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

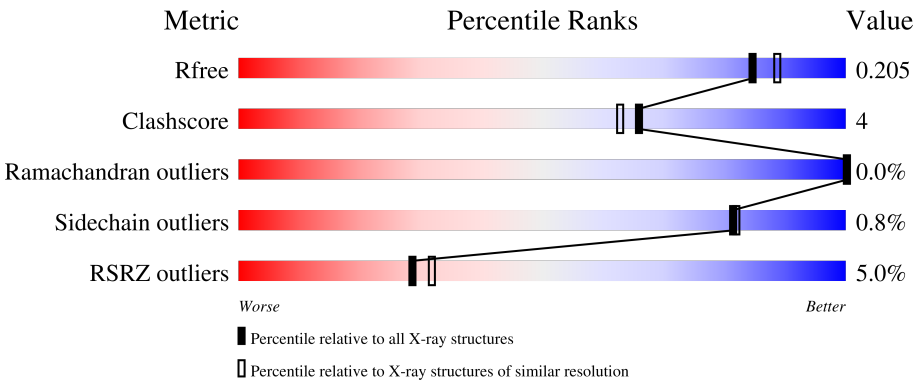
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.37.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.37.1 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 6207 (1.90-1.90) |
| Clashscore | 141614 | 6847 (1.90-1.90) |
| Ramachandran outliers | 138981 | 6760 (1.90-1.90) |
| Sidechain outliers | 138945 | 6760 (1.90-1.90) |
| RSRZ outliers | 127900 | 6082 (1.90-1.90) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 611 | .% 87% 5% 8% |
| 1 | B | 611 | .% 88% • 8% |
| 1 | C | 611 | .% 86% 5% 8% |
| 1 | D | 611 | .% 88% • 8% |
| 1 | E | 611 | 85% 7% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 611 | %, 87%, 5%, 8% |
| 1 | G | 611 | %, 85%, 7%, 8% |
| 1 | H | 611 | 4%, 84%, 8%, 8% |
| 1 | I | 611 | 16%, 82%, 9%, 8% |
| 1 | J | 611 | 22%, 73%, 18%, 8% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47549 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 562 | 4147 | 2597 | 729 | 793 | 28 | 0 | 0 | 0 |
| 1 | B | 561 | 4140 | 2592 | 728 | 792 | 28 | 0 | 0 | 0 |
| 1 | C | 561 | 4140 | 2592 | 728 | 792 | 28 | 0 | 0 | 0 |
| 1 | D | 561 | 4140 | 2592 | 728 | 792 | 28 | 0 | 0 | 0 |
| 1 | E | 561 | 4140 | 2592 | 728 | 792 | 28 | 0 | 0 | 0 |
| 1 | F | 561 | 4140 | 2592 | 728 | 792 | 28 | 0 | 0 | 0 |
| 1 | G | 562 | 4147 | 2597 | 729 | 793 | 28 | 0 | 0 | 0 |
| 1 | H | 562 | 4147 | 2597 | 729 | 793 | 28 | 0 | 0 | 0 |
| 1 | I | 561 | 4140 | 2592 | 728 | 792 | 28 | 0 | 0 | 0 |
| 1 | J | 560 | 4133 | 2587 | 727 | 791 | 28 | 0 | 0 | 0 |

There are 80 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| A | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| A | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| A | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| A | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| A | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| A | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| A | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| B | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| B | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| B | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| B | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| B | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| B | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| B | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| C | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| C | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| C | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| C | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| C | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| C | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| C | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| C | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| D | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| D | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| D | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| D | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| D | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| D | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| D | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| D | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| E | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| E | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| E | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| E | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| E | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| E | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| E | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| E | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| F | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| F | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| F | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| F | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| F | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| F | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| F | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| F | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| G | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| G | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| G | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| G | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| G | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| G | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| G | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| H | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| H | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| H | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| H | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| H | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| H | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| H | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| H | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| I | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| I | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| I | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| I | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| I | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| I | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| I | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| I | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| J | 604 | LEU | - | expression tag | UNP A0A0K8P8E7 |
| J | 605 | GLU | - | expression tag | UNP A0A0K8P8E7 |
| J | 606 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| J | 607 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| J | 608 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| J | 609 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| J | 610 | HIS | - | expression tag | UNP A0A0K8P8E7 |
| J | 611 | HIS | - | expression tag | UNP A0A0K8P8E7 |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Ca | | |
| 2 | A | 1 | 1 | 1 | 0 | 0 |
| 2 | B | 1 | 1 | 1 | 0 | 0 |
| 2 | C | 1 | 1 | 1 | 0 | 0 |
| 2 | D | 1 | 1 | 1 | 0 | 0 |
| 2 | E | 1 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | F | 1 | Total Ca<br>1 1 | 0 | 0 |
| 2 | G | 1 | Total Ca<br>1 1 | 0 | 0 |
| 2 | H | 1 | Total Ca<br>1 1 | 0 | 0 |
| 2 | I | 1 | Total Ca<br>1 1 | 0 | 0 |
| 2 | J | 1 | Total Ca<br>1 1 | 0 | 0 |

- Molecule 3 is water.

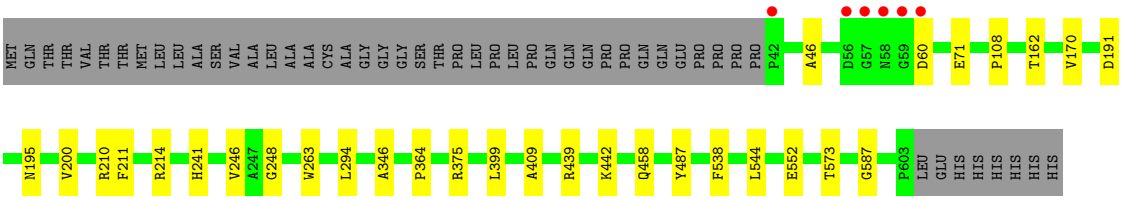
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 777 | Total O<br>777 777 | 0 | 0 |
| 3 | B | 759 | Total O<br>759 759 | 0 | 0 |
| 3 | C | 785 | Total O<br>785 785 | 0 | 0 |
| 3 | D | 706 | Total O<br>706 706 | 0 | 0 |
| 3 | E | 724 | Total O<br>724 724 | 0 | 0 |
| 3 | F | 773 | Total O<br>773 773 | 0 | 0 |
| 3 | G | 567 | Total O<br>567 567 | 0 | 0 |
| 3 | H | 461 | Total O<br>461 461 | 0 | 0 |
| 3 | I | 341 | Total O<br>341 341 | 0 | 0 |
| 3 | J | 232 | Total O<br>232 232 | 0 | 0 |

# 3 Residue-property plots (i)

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

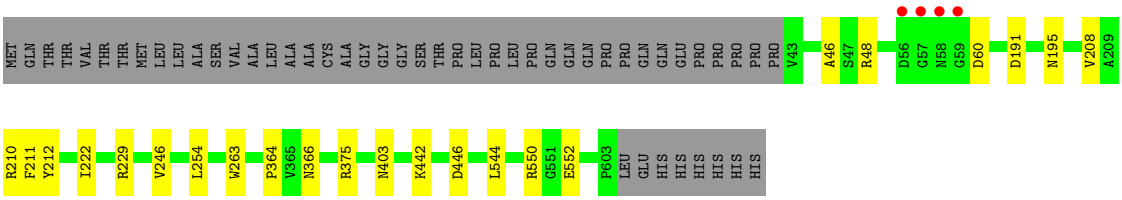
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain A:



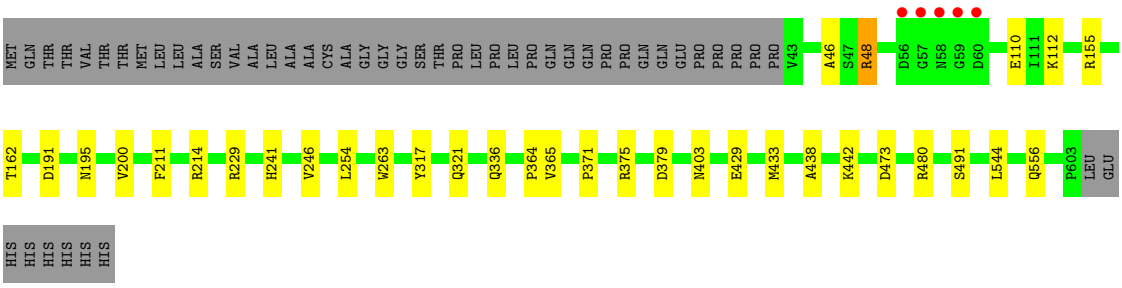

• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain B:



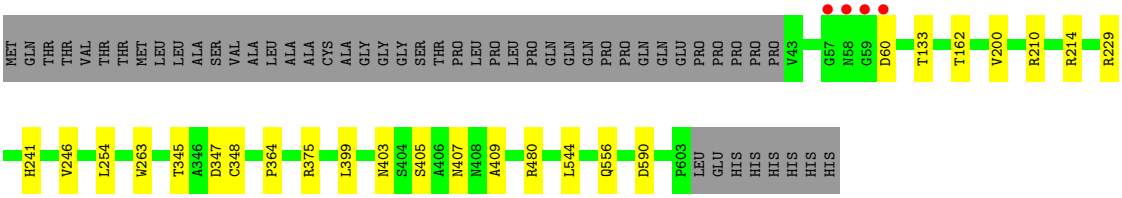

• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain C:



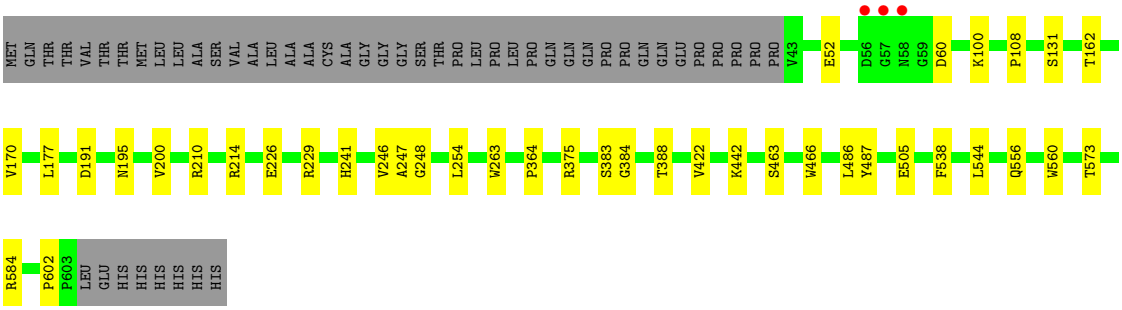

• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain D:



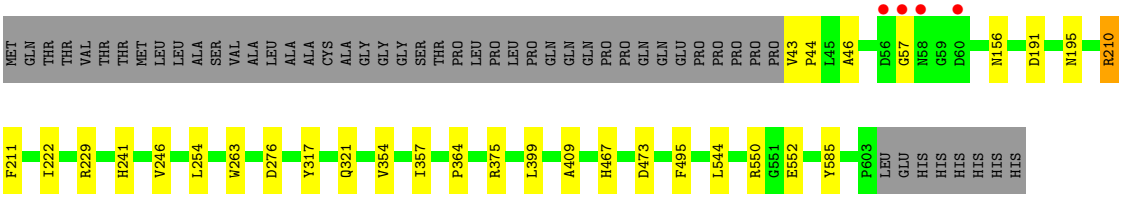

- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain E:



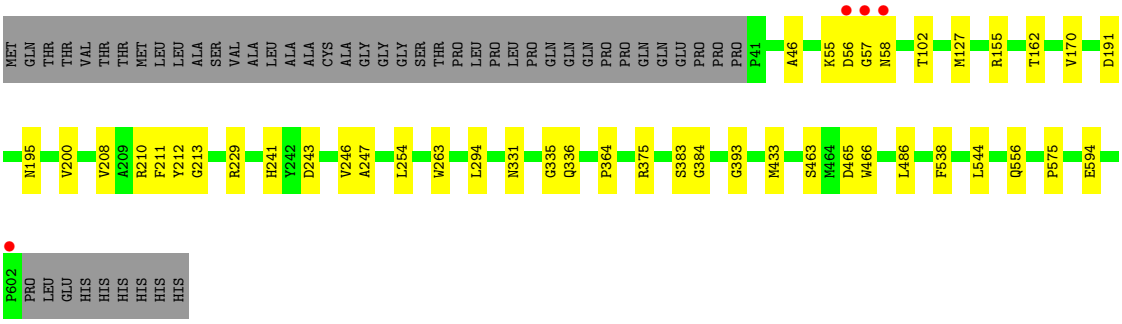

- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain F:



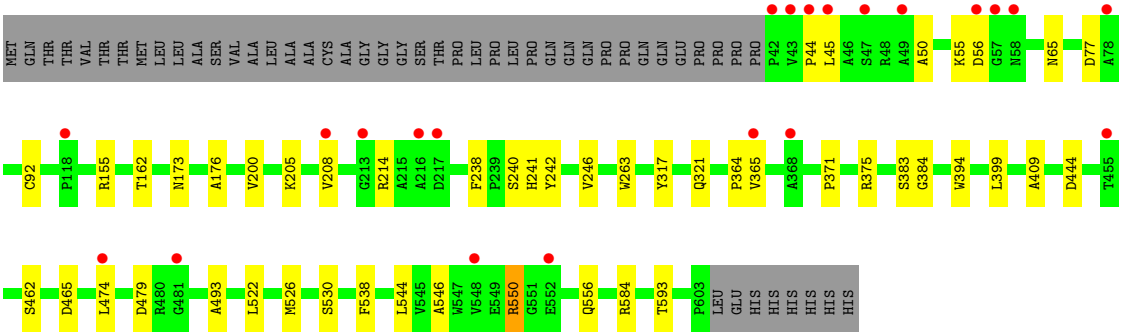

- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain G:



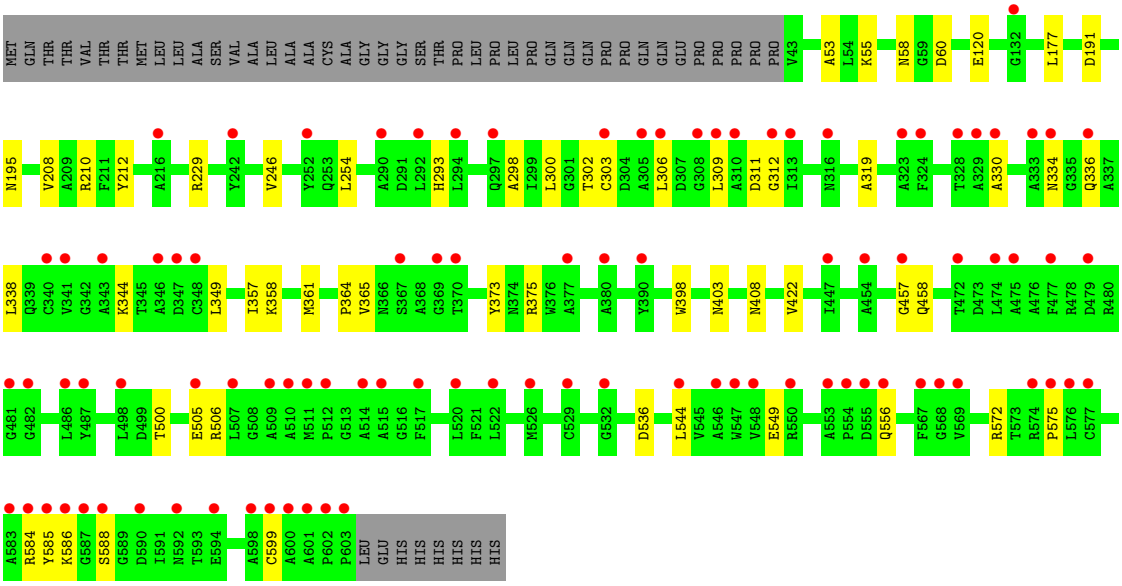

- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain H:



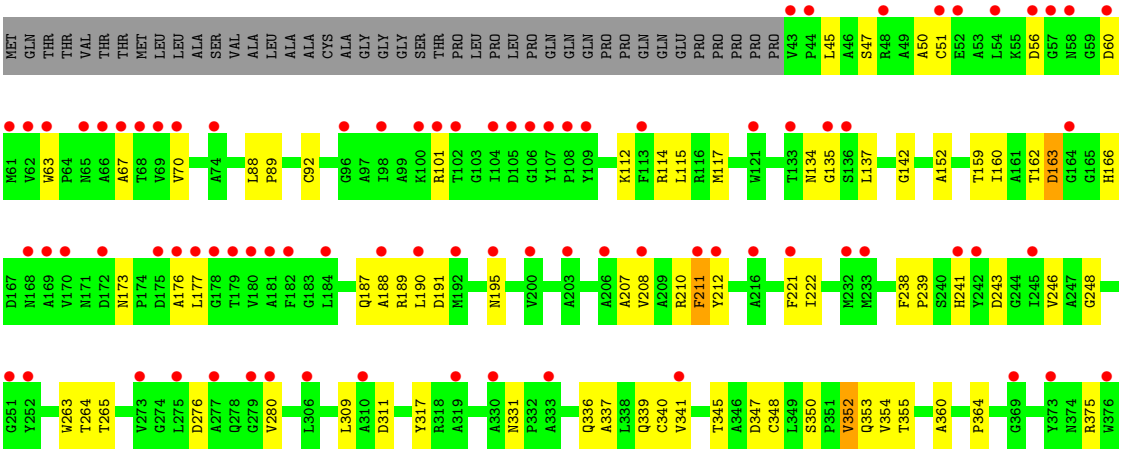

• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

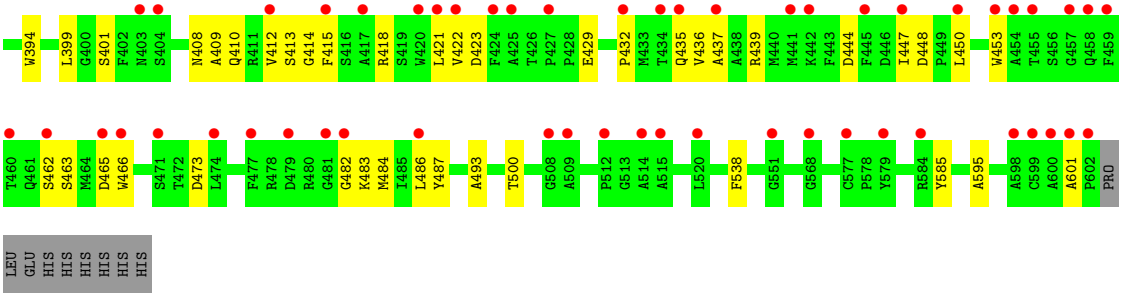
Chain I:




• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain J:




W394
L399
G400
S401
F402
N403
S404
N408
A409
Q410
R411
V412
S413
G414
F415
S416
A417
R418
S419
W420
L421
V422
D423
F424
A425
T426
P427
P428
E429
P432
M433
T434
Q435
V436
A437
A438
R439
M440
M441
K442
F443
D444
F445
D446
I447
D448
P449
L450
W453
A454
T455
S456
G457
Q458
F459
T460
Q461
S462
S463
M464
D465
W466
S471
T472
D473
L474
F477
R478
D479
R480
G481
G482
K483
M484
I485
L486
Y487
A493
T500
G508
A509
P512
G513
A514
A515
L520
F538
G551
G568
C577
P578
Y579
R584
Y585
A595
A598
C599
A600
A601
P602
PRO
LEU
GLU
HIS
HIS
HIS
HIS
HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 110.49Å 135.63Å 138.15Å<br>83.09° 67.91° 67.57° | Depositor |
| Resolution (Å) | 57.62 – 1.90<br>88.35 – 1.90 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 93.6 (57.62-1.90)<br>93.7 (88.35-1.90) | Depositor<br>EDS |
| $R_{merge}$ | 0.06 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.29 (at 1.90Å) | Xtriage |
| Refinement program | PHENIX (1.13_2998: ???) | Depositor |
| R, $R_{free}$ | 0.185 , 0.205<br>0.185 , 0.205 | Depositor<br>DCC |
| $R_{free}$ test set | 24892 reflections (4.91%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 21.8 | Xtriage |
| Anisotropy | 0.116 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 47.4 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | 0.016 for h,l,h-k<br>0.016 for h,h-l,k<br>0.023 for h,h-k,h-l<br>0.017 for -h,-h+k,-l<br>0.017 for -h,-k,-h+l<br>0.023 for -h,-l,-k<br>0.055 for -h,-h+l,-h+k | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 47549 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 28.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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 | 0.26 | 0/4256 | 0.46 | 0/5796 |
| 1 | B | 0.27 | 0/4248 | 0.47 | 0/5785 |
| 1 | C | 0.27 | 0/4248 | 0.47 | 0/5785 |
| 1 | D | 0.26 | 0/4248 | 0.47 | 0/5785 |
| 1 | E | 0.26 | 0/4248 | 0.46 | 0/5785 |
| 1 | F | 0.26 | 0/4248 | 0.47 | 0/5785 |
| 1 | G | 0.26 | 0/4256 | 0.45 | 0/5796 |
| 1 | H | 0.26 | 0/4256 | 0.46 | 0/5796 |
| 1 | I | 0.28 | 0/4248 | 0.47 | 0/5785 |
| 1 | J | 0.28 | 0/4240 | 0.49 | 0/5773 |
| All | All | 0.27 | 0/42496 | 0.47 | 0/57871 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 4147 | 0 | 3937 | 19 | 0 |
| 1 | B | 4140 | 0 | 3929 | 16 | 0 |
| 1 | C | 4140 | 0 | 3929 | 22 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | D | 4140 | 0 | 3929 | 24 | 0 |
| 1 | E | 4140 | 0 | 3929 | 27 | 0 |
| 1 | F | 4140 | 0 | 3929 | 22 | 0 |
| 1 | G | 4147 | 0 | 3937 | 31 | 0 |
| 1 | H | 4147 | 0 | 3937 | 32 | 0 |
| 1 | I | 4140 | 0 | 3929 | 50 | 0 |
| 1 | J | 4133 | 0 | 3922 | 85 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 2 | E | 1 | 0 | 0 | 0 | 0 |
| 2 | F | 1 | 0 | 0 | 0 | 0 |
| 2 | G | 1 | 0 | 0 | 0 | 0 |
| 2 | H | 1 | 0 | 0 | 0 | 0 |
| 2 | I | 1 | 0 | 0 | 0 | 0 |
| 2 | J | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 777 | 0 | 0 | 7 | 4 |
| 3 | B | 759 | 0 | 0 | 7 | 1 |
| 3 | C | 785 | 0 | 0 | 11 | 3 |
| 3 | D | 706 | 0 | 0 | 14 | 3 |
| 3 | E | 724 | 0 | 0 | 14 | 8 |
| 3 | F | 773 | 0 | 0 | 8 | 1 |
| 3 | G | 567 | 0 | 0 | 16 | 4 |
| 3 | H | 461 | 0 | 0 | 14 | 3 |
| 3 | I | 341 | 0 | 0 | 25 | 0 |
| 3 | J | 232 | 0 | 0 | 29 | 1 |
| All | All | 47549 | 0 | 39307 | 326 | 14 |

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 4.

All (326) 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:H:92:CYS:SG | 3:H:1295:HOH:O | 2.21 | 0.98 |
| 1:J:345:THR:HG23 | 1:J:347:ASP:H | 1.26 | 0.98 |
| 1:E:602:PRO:O | 3:E:901:HOH:O | 1.87 | 0.91 |
| 1:G:58:ASN:N | 3:G:901:HOH:O | 2.02 | 0.90 |
| 1:F:57:GLY:N | 3:F:902:HOH:O | 2.05 | 0.89 |
| 1:D:345:THR:HG23 | 1:D:347:ASP:H | 1.37 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:549:GLU:OE2 | 3:I:901:HOH:O | 1.93 | 0.86 |
| 1:J:117:MET:SD | 3:J:1108:HOH:O | 2.33 | 0.86 |
| 1:I:336:GLN:NE2 | 3:I:902:HOH:O | 1.94 | 0.85 |
| 1:F:354:VAL:O | 3:F:901:HOH:O | 1.96 | 0.84 |
| 1:B:442:LYS:CE | 3:B:924:HOH:O | 2.26 | 0.83 |
| 1:J:317:TYR:OH | 3:J:901:HOH:O | 1.96 | 0.82 |
| 1:D:405:SER:OG | 3:D:901:HOH:O | 1.86 | 0.82 |
| 1:J:422:VAL:O | 3:J:902:HOH:O | 1.97 | 0.81 |
| 1:I:588:SER:O | 3:I:904:HOH:O | 1.98 | 0.81 |
| 1:E:131:SER:HA | 3:E:907:HOH:O | 1.83 | 0.79 |
| 1:I:536:ASP:OD2 | 3:I:903:HOH:O | 1.97 | 0.79 |
| 1:C:473:ASP:OD2 | 3:C:902:HOH:O | 1.99 | 0.79 |
| 1:D:60:ASP:O | 1:D:210:ARG:NH2 | 2.16 | 0.79 |
| 1:J:473:ASP:OD1 | 3:J:903:HOH:O | 2.01 | 0.79 |
| 1:J:101:ARG:NE | 3:J:912:HOH:O | 2.17 | 0.77 |
| 1:J:190:LEU:N | 3:J:910:HOH:O | 2.16 | 0.76 |
| 1:J:177:LEU:HD12 | 1:J:422:VAL:HG23 | 1.66 | 0.76 |
| 1:J:221:PHE:O | 3:J:904:HOH:O | 2.04 | 0.75 |
| 1:C:48:ARG:NH1 | 3:C:901:HOH:O | 1.90 | 0.75 |
| 1:H:526:MET:HE2 | 1:H:530:SER:HA | 1.69 | 0.74 |
| 1:J:337:ALA:O | 3:J:905:HOH:O | 2.06 | 0.73 |
| 1:I:506:ARG:NH1 | 3:I:915:HOH:O | 2.22 | 0.73 |
| 1:G:55:LYS:O | 3:G:901:HOH:O | 2.05 | 0.73 |
| 1:H:77:ASP:O | 3:H:901:HOH:O | 2.06 | 0.73 |
| 1:H:45:LEU:O | 3:H:902:HOH:O | 2.06 | 0.73 |
| 1:G:56:ASP:OD2 | 3:G:903:HOH:O | 2.06 | 0.73 |
| 1:G:393:GLY:HA3 | 3:G:1138:HOH:O | 1.88 | 0.72 |
| 1:G:335:GLY:O | 3:G:902:HOH:O | 2.06 | 0.72 |
| 1:H:546:ALA:HA | 1:H:550:ARG:HH21 | 1.56 | 0.71 |
| 1:J:246:VAL:N | 3:J:904:HOH:O | 2.18 | 0.71 |
| 1:I:120:GLU:OE2 | 3:I:905:HOH:O | 2.08 | 0.70 |
| 1:J:191:ASP:HA | 1:J:195:ASN:HB3 | 1.74 | 0.70 |
| 1:I:556:GLN:HG2 | 1:I:599:CYS:SG | 2.31 | 0.70 |
| 1:J:340:CYS:O | 3:J:907:HOH:O | 2.09 | 0.69 |
| 1:I:229:ARG:HD3 | 1:I:254:LEU:HD12 | 1.72 | 0.69 |
| 1:C:429:GLU:OE2 | 3:C:903:HOH:O | 2.10 | 0.69 |
| 1:G:213:GLY:N | 3:G:905:HOH:O | 2.19 | 0.69 |
| 1:F:585:TYR:OH | 3:F:903:HOH:O | 2.10 | 0.69 |
| 1:E:226:GLU:N | 3:E:907:HOH:O | 2.26 | 0.67 |
| 1:I:303:CYS:HA | 1:I:306:LEU:HD13 | 1.75 | 0.67 |
| 1:F:473:ASP:OD1 | 3:F:904:HOH:O | 2.13 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:345:THR:HG23 | 1:J:347:ASP:N | 2.04 | 0.67 |
| 1:B:403:ASN:OD1 | 3:B:901:HOH:O | 2.10 | 0.67 |
| 1:J:429:GLU:OE1 | 3:J:908:HOH:O | 2.13 | 0.67 |
| 1:I:330:ALA:O | 3:I:906:HOH:O | 2.12 | 0.67 |
| 1:A:71:GLU:OE2 | 3:A:903:HOH:O | 2.11 | 0.67 |
| 1:H:479:ASP:OD2 | 3:H:904:HOH:O | 2.13 | 0.66 |
| 1:D:407:ASN:ND2 | 3:D:905:HOH:O | 2.28 | 0.66 |
| 1:G:556:GLN:OE1 | 3:G:904:HOH:O | 2.13 | 0.66 |
| 1:I:408:ASN:O | 3:I:907:HOH:O | 2.13 | 0.66 |
| 1:I:457:GLY:HA3 | 3:I:931:HOH:O | 1.95 | 0.66 |
| 1:B:550:ARG:HB2 | 1:B:552:GLU:HG3 | 1.78 | 0.66 |
| 1:J:500:THR:OG1 | 3:J:906:HOH:O | 2.09 | 0.66 |
| 1:C:403:ASN:ND2 | 3:C:909:HOH:O | 2.24 | 0.66 |
| 1:J:115:LEU:HB2 | 1:J:160:ILE:HD13 | 1.78 | 0.66 |
| 1:I:549:GLU:O | 3:I:908:HOH:O | 2.14 | 0.66 |
| 1:C:556:GLN:NE2 | 3:C:914:HOH:O | 2.29 | 0.66 |
| 1:E:388:THR:N | 3:E:902:HOH:O | 1.92 | 0.66 |
| 1:B:442:LYS:HE3 | 3:B:924:HOH:O | 1.89 | 0.65 |
| 1:E:214:ARG:NH1 | 3:E:903:HOH:O | 2.00 | 0.65 |
| 1:J:56:ASP:OD1 | 3:J:909:HOH:O | 2.15 | 0.65 |
| 1:G:246:VAL:HG23 | 1:G:544:LEU:HD22 | 1.77 | 0.65 |
| 1:J:409:ALA:HB3 | 1:J:412:VAL:HG22 | 1.79 | 0.64 |
| 1:B:210:ARG:NH1 | 3:B:903:HOH:O | 2.28 | 0.64 |
| 1:D:246:VAL:HG23 | 1:D:544:LEU:HD22 | 1.79 | 0.64 |
| 1:B:60:ASP:O | 3:B:903:HOH:O | 2.16 | 0.64 |
| 1:F:357:ILE:N | 3:F:901:HOH:O | 2.30 | 0.64 |
| 1:J:345:THR:HG22 | 1:J:348:CYS:SG | 2.38 | 0.64 |
| 1:B:229:ARG:HD3 | 1:B:254:LEU:HD12 | 1.80 | 0.63 |
| 1:C:336:GLN:OE1 | 3:C:906:HOH:O | 2.16 | 0.63 |
| 1:D:214:ARG:NE | 3:D:903:HOH:O | 2.23 | 0.63 |
| 1:E:229:ARG:HD3 | 1:E:254:LEU:HD12 | 1.81 | 0.63 |
| 1:C:473:ASP:OD1 | 3:C:905:HOH:O | 2.15 | 0.63 |
| 1:I:584:ARG:HH22 | 1:I:586:LYS:HA | 1.64 | 0.63 |
| 1:J:188:ALA:C | 3:J:910:HOH:O | 2.36 | 0.63 |
| 1:J:309:LEU:HD12 | 1:J:585:TYR:HB2 | 1.81 | 0.63 |
| 1:I:309:LEU:HD12 | 1:I:585:TYR:HB2 | 1.81 | 0.62 |
| 1:G:229:ARG:HD3 | 1:G:254:LEU:HD12 | 1.82 | 0.62 |
| 1:E:505:GLU:OE1 | 3:E:904:HOH:O | 2.16 | 0.62 |
| 1:I:246:VAL:HG23 | 1:I:544:LEU:HD22 | 1.81 | 0.62 |
| 1:J:191:ASP:N | 3:J:910:HOH:O | 2.33 | 0.62 |
| 1:A:458:GLN:NE2 | 3:A:912:HOH:O | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:246:VAL:HG23 | 1:E:544:LEU:HD22 | 1.82 | 0.62 |
| 1:J:309:LEU:HD22 | 1:J:311:ASP:HB3 | 1.82 | 0.61 |
| 1:I:458:GLN:NE2 | 3:I:924:HOH:O | 2.33 | 0.61 |
| 1:D:214:ARG:NH2 | 3:D:903:HOH:O | 2.17 | 0.61 |
| 1:B:48:ARG:NH2 | 3:B:902:HOH:O | 2.11 | 0.60 |
| 1:F:246:VAL:HG23 | 1:F:544:LEU:HD22 | 1.83 | 0.60 |
| 1:H:546:ALA:HA | 1:H:550:ARG:NH2 | 2.15 | 0.60 |
| 1:I:364:PRO:O | 3:I:909:HOH:O | 2.17 | 0.59 |
| 1:C:155:ARG:NH1 | 3:C:918:HOH:O | 2.34 | 0.59 |
| 1:G:336:GLN:NE2 | 3:G:914:HOH:O | 2.35 | 0.59 |
| 1:F:550:ARG:NH1 | 3:F:911:HOH:O | 2.34 | 0.59 |
| 1:A:214:ARG:NH2 | 3:A:907:HOH:O | 2.26 | 0.59 |
| 1:E:210:ARG:NH1 | 3:E:911:HOH:O | 2.36 | 0.59 |
| 1:J:453:TRP:O | 3:J:911:HOH:O | 2.17 | 0.59 |
| 1:J:47:SER:H | 1:J:211:PHE:HE1 | 1.49 | 0.59 |
| 1:D:590:ASP:OD2 | 3:D:902:HOH:O | 2.16 | 0.58 |
| 1:A:294:LEU:HD11 | 1:A:346:ALA:O | 2.03 | 0.58 |
| 1:B:246:VAL:HG23 | 1:B:544:LEU:HD22 | 1.86 | 0.58 |
| 1:A:60:ASP:O | 1:A:210:ARG:NH2 | 2.35 | 0.58 |
| 1:E:247:ALA:HB3 | 1:E:486:LEU:HD23 | 1.84 | 0.58 |
| 1:J:462:SER:HB3 | 1:J:465:ASP:HB2 | 1.85 | 0.58 |
| 1:D:556:GLN:NE2 | 3:D:909:HOH:O | 2.37 | 0.58 |
| 1:A:246:VAL:HG23 | 1:A:544:LEU:HD22 | 1.87 | 0.57 |
| 1:C:214:ARG:NH1 | 3:C:920:HOH:O | 2.37 | 0.57 |
| 1:A:573:THR:HB | 3:A:1168:HOH:O | 2.04 | 0.57 |
| 1:F:222:ILE:HG12 | 1:F:246:VAL:HB | 1.86 | 0.56 |
| 1:I:584:ARG:HG2 | 1:I:584:ARG:HH21 | 1.70 | 0.56 |
| 1:H:321:GLN:O | 3:H:905:HOH:O | 2.18 | 0.56 |
| 1:D:214:ARG:NH1 | 3:D:910:HOH:O | 2.37 | 0.56 |
| 1:F:229:ARG:NE | 1:F:467:HIS:CE1 | 2.74 | 0.56 |
| 1:J:173:ASN:HB3 | 1:J:176:ALA:HB3 | 1.87 | 0.56 |
| 1:D:345:THR:HG22 | 1:D:348:CYS:SG | 2.45 | 0.55 |
| 1:D:214:ARG:NH2 | 3:D:910:HOH:O | 2.39 | 0.55 |
| 1:I:60:ASP:OD1 | 1:I:210:ARG:NH2 | 2.38 | 0.55 |
| 1:J:189:ARG:NE | 3:J:902:HOH:O | 2.27 | 0.55 |
| 1:H:205:LYS:HA | 1:H:208:VAL:HG22 | 1.87 | 0.55 |
| 1:H:214:ARG:HD2 | 3:H:916:HOH:O | 2.07 | 0.55 |
| 1:E:226:GLU:HB3 | 3:E:907:HOH:O | 2.07 | 0.55 |
| 1:J:412:VAL:HG23 | 1:J:413:SER:H | 1.72 | 0.55 |
| 1:C:246:VAL:HG23 | 1:C:544:LEU:HD22 | 1.89 | 0.54 |
| 1:H:556:GLN:O | 3:H:906:HOH:O | 2.19 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:306:LEU:HD23 | 1:I:319:ALA:HB1 | 1.89 | 0.53 |
| 1:J:177:LEU:HD22 | 1:J:418:ARG:HG2 | 1.90 | 0.53 |
| 1:D:403:ASN:ND2 | 3:D:914:HOH:O | 2.40 | 0.53 |
| 1:E:556:GLN:NE2 | 3:E:905:HOH:O | 2.21 | 0.53 |
| 1:J:177:LEU:HD12 | 1:J:422:VAL:CG2 | 2.37 | 0.53 |
| 1:I:338:LEU:O | 1:I:349:LEU:N | 2.42 | 0.53 |
| 1:E:442:LYS:HE2 | 3:E:1188:HOH:O | 2.09 | 0.53 |
| 1:I:584:ARG:NH2 | 1:I:585:TYR:O | 2.42 | 0.53 |
| 1:F:276:ASP:HB2 | 3:F:1330:HOH:O | 2.08 | 0.52 |
| 1:I:311:ASP:HB2 | 1:I:572:ARG:HH12 | 1.75 | 0.52 |
| 1:C:229:ARG:HD3 | 1:C:254:LEU:HD12 | 1.91 | 0.52 |
| 1:E:100:LYS:HG3 | 3:E:1284:HOH:O | 2.10 | 0.52 |
| 1:C:438:ALA:O | 1:C:442:LYS:HG3 | 2.09 | 0.52 |
| 1:G:247:ALA:HB3 | 1:G:486:LEU:HD23 | 1.92 | 0.52 |
| 1:A:552:GLU:OE2 | 3:A:905:HOH:O | 2.19 | 0.52 |
| 1:H:246:VAL:HG23 | 1:H:544:LEU:HD22 | 1.92 | 0.52 |
| 1:F:254:LEU:HD21 | 1:F:495:PHE:CZ | 2.45 | 0.52 |
| 1:J:67:ALA:O | 3:J:914:HOH:O | 2.19 | 0.52 |
| 1:A:214:ARG:NH1 | 3:A:902:HOH:O | 2.10 | 0.51 |
| 1:J:187:GLN:O | 3:J:910:HOH:O | 2.19 | 0.51 |
| 1:D:133:THR:HG23 | 3:D:923:HOH:O | 2.10 | 0.51 |
| 1:J:601:ALA:HB1 | 3:J:933:HOH:O | 2.11 | 0.51 |
| 1:G:465:ASP:O | 3:G:906:HOH:O | 2.19 | 0.51 |
| 1:H:162:THR:HB | 1:H:200:VAL:HG21 | 1.93 | 0.50 |
| 1:I:344:LYS:HZ1 | 1:I:349:LEU:HA | 1.75 | 0.50 |
| 1:J:421:LEU:HD21 | 1:J:439:ARG:HG2 | 1.92 | 0.50 |
| 1:G:393:GLY:CA | 3:G:1138:HOH:O | 2.51 | 0.50 |
| 1:H:242:TYR:N | 3:H:903:HOH:O | 2.12 | 0.50 |
| 1:J:92:CYS:CB | 1:J:211:PHE:HE2 | 2.24 | 0.50 |
| 1:C:403:ASN:ND2 | 3:C:924:HOH:O | 2.44 | 0.50 |
| 1:I:55:LYS:HE3 | 3:I:1108:HOH:O | 2.12 | 0.50 |
| 1:D:556:GLN:NE2 | 3:D:912:HOH:O | 2.39 | 0.50 |
| 1:I:365:VAL:O | 3:I:911:HOH:O | 2.19 | 0.50 |
| 1:J:447:ILE:HA | 1:J:450:LEU:HD12 | 1.93 | 0.50 |
| 1:H:444:ASP:OD2 | 3:H:908:HOH:O | 2.20 | 0.50 |
| 1:J:135:GLY:HA2 | 1:J:166:HIS:O | 2.12 | 0.49 |
| 1:J:264:THR:HG22 | 1:J:360:ALA:HB1 | 1.95 | 0.49 |
| 1:E:60:ASP:CB | 1:E:210:ARG:HH12 | 2.26 | 0.49 |
| 1:E:162:THR:HB | 1:E:200:VAL:HG21 | 1.94 | 0.48 |
| 1:I:309:LEU:HD22 | 1:I:311:ASP:HB3 | 1.93 | 0.48 |
| 1:A:108:PRO:HG2 | 1:A:170:VAL:HG11 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:439:ARG:HA | 1:A:442:LYS:HE3 | 1.96 | 0.48 |
| 1:A:263:TRP:CD2 | 1:A:364:PRO:HA | 2.49 | 0.48 |
| 1:J:222:ILE:HG12 | 1:J:246:VAL:HB | 1.95 | 0.48 |
| 1:J:399:LEU:C | 1:J:409:ALA:HB2 | 2.33 | 0.48 |
| 1:G:383:SER:OG | 1:G:384:GLY:N | 2.47 | 0.48 |
| 1:J:208:VAL:HA | 3:J:1108:HOH:O | 2.14 | 0.48 |
| 1:J:63:TRP:CH2 | 1:J:207:ALA:HB2 | 2.49 | 0.48 |
| 1:I:373:TYR:OH | 3:I:912:HOH:O | 2.20 | 0.48 |
| 1:F:263:TRP:CD2 | 1:F:364:PRO:HA | 2.49 | 0.47 |
| 1:E:442:LYS:HG2 | 3:E:1188:HOH:O | 2.13 | 0.47 |
| 1:C:480:ARG:NH2 | 3:C:904:HOH:O | 2.14 | 0.47 |
| 1:E:52:GLU:HG3 | 3:E:1023:HOH:O | 2.14 | 0.47 |
| 1:F:156:ASN:ND2 | 3:F:925:HOH:O | 2.47 | 0.47 |
| 1:G:208:VAL:HG13 | 1:G:212:TYR:HD2 | 1.78 | 0.47 |
| 1:I:575:PRO:O | 3:I:913:HOH:O | 2.20 | 0.47 |
| 1:G:210:ARG:C | 3:G:905:HOH:O | 2.52 | 0.47 |
| 1:J:263:TRP:CD2 | 1:J:364:PRO:HA | 2.50 | 0.47 |
| 1:H:263:TRP:HB2 | 1:H:364:PRO:HB3 | 1.95 | 0.47 |
| 1:H:263:TRP:CD2 | 1:H:364:PRO:HA | 2.50 | 0.47 |
| 1:J:45:LEU:HD23 | 1:J:212:TYR:O | 2.15 | 0.47 |
| 1:D:263:TRP:CD2 | 1:D:364:PRO:HA | 2.50 | 0.47 |
| 1:H:474:LEU:HA | 3:H:1141:HOH:O | 2.13 | 0.47 |
| 1:H:55:LYS:HE3 | 1:H:56:ASP:HB2 | 1.97 | 0.47 |
| 1:E:383:SER:OG | 1:E:384:GLY:N | 2.46 | 0.46 |
| 1:I:293:HIS:CE1 | 3:I:935:HOH:O | 2.68 | 0.46 |
| 1:I:506:ARG:CZ | 3:I:915:HOH:O | 2.62 | 0.46 |
| 1:D:162:THR:HB | 1:D:200:VAL:HG21 | 1.96 | 0.46 |
| 1:A:162:THR:HB | 1:A:200:VAL:HG21 | 1.97 | 0.46 |
| 1:D:480:ARG:NH2 | 3:D:904:HOH:O | 2.19 | 0.46 |
| 1:J:88:LEU:HA | 1:J:89:PRO:HD3 | 1.80 | 0.46 |
| 1:J:595:ALA:HB2 | 3:J:987:HOH:O | 2.15 | 0.46 |
| 1:H:44:PRO:O | 1:H:50:ALA:HB2 | 2.16 | 0.46 |
| 1:C:110:GLU:OE2 | 1:C:112:LYS:NZ | 2.45 | 0.46 |
| 1:C:162:THR:HB | 1:C:200:VAL:HG21 | 1.97 | 0.46 |
| 1:D:210:ARG:HH21 | 1:F:210:ARG:HH12 | 1.63 | 0.46 |
| 1:I:300:LEU:HD22 | 1:I:312:GLY:HA2 | 1.96 | 0.46 |
| 1:I:344:LYS:NZ | 1:I:349:LEU:HA | 2.32 | 0.45 |
| 1:J:401:SER:N | 1:J:408:ASN:OD1 | 2.46 | 0.45 |
| 1:B:46:ALA:HA | 1:B:211:PHE:CZ | 2.51 | 0.45 |
| 1:C:46:ALA:HA | 1:C:211:PHE:CZ | 2.52 | 0.45 |
| 1:J:114:ARG:O | 1:J:160:ILE:HD12 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:560:TRP:HB3 | 1:E:573:THR:HG22 | 1.99 | 0.45 |
| 1:H:462:SER:O | 1:H:465:ASP:HB2 | 2.16 | 0.45 |
| 1:J:56:ASP:OD2 | 1:J:70:VAL:N | 2.48 | 0.45 |
| 1:J:248:GLY:HA3 | 1:J:487:TYR:CZ | 2.51 | 0.45 |
| 1:D:229:ARG:HD3 | 1:D:254:LEU:HD12 | 1.98 | 0.45 |
| 1:H:593:THR:HG21 | 3:H:1283:HOH:O | 2.17 | 0.45 |
| 1:I:53:ALA:HB3 | 3:I:971:HOH:O | 2.16 | 0.45 |
| 1:J:412:VAL:HG23 | 1:J:413:SER:N | 2.30 | 0.45 |
| 1:F:550:ARG:HB2 | 1:F:552:GLU:HG3 | 1.99 | 0.45 |
| 1:G:433:MET:HG3 | 3:G:1098:HOH:O | 2.16 | 0.45 |
| 1:H:65:ASN:HB2 | 3:H:1139:HOH:O | 2.16 | 0.44 |
| 1:I:298:ALA:O | 1:I:302:THR:HG23 | 2.17 | 0.44 |
| 1:I:500:THR:HG22 | 3:I:996:HOH:O | 2.16 | 0.44 |
| 1:J:162:THR:OG1 | 1:J:163:ASP:N | 2.50 | 0.44 |
| 1:J:238:PHE:HB3 | 1:J:241:HIS:CD2 | 2.52 | 0.44 |
| 1:I:505:GLU:OE2 | 3:I:914:HOH:O | 2.21 | 0.44 |
| 1:C:317:TYR:O | 1:C:321:GLN:HG2 | 2.18 | 0.44 |
| 1:D:210:ARG:NH1 | 3:D:938:HOH:O | 2.51 | 0.44 |
| 1:G:57:GLY:N | 3:G:901:HOH:O | 2.49 | 0.44 |
| 1:I:357:ILE:O | 1:I:361:MET:HG2 | 2.18 | 0.44 |
| 1:J:423:ASP:HA | 3:J:902:HOH:O | 2.17 | 0.44 |
| 1:G:243:ASP:HA | 3:G:938:HOH:O | 2.17 | 0.44 |
| 1:H:394:TRP:CD1 | 1:H:493:ALA:HB2 | 2.53 | 0.44 |
| 1:J:341:VAL:C | 3:J:907:HOH:O | 2.55 | 0.44 |
| 1:G:191:ASP:HA | 1:G:195:ASN:HB3 | 2.00 | 0.44 |
| 1:G:46:ALA:HA | 1:G:211:PHE:CZ | 2.52 | 0.44 |
| 1:A:587:GLY:O | 1:G:170:VAL:HG22 | 2.18 | 0.43 |
| 1:G:162:THR:HB | 1:G:200:VAL:HG21 | 2.00 | 0.43 |
| 1:D:214:ARG:CZ | 3:D:910:HOH:O | 2.66 | 0.43 |
| 1:F:263:TRP:HB2 | 1:F:364:PRO:HB3 | 2.00 | 0.43 |
| 1:J:331:ASN:N | 1:J:336:GLN:O | 2.47 | 0.43 |
| 1:J:410:GLN:OE1 | 1:J:415:PHE:HB2 | 2.18 | 0.43 |
| 1:J:410:GLN:HA | 1:J:414:GLY:HA3 | 2.00 | 0.43 |
| 1:J:483:LYS:NZ | 3:J:919:HOH:O | 2.27 | 0.43 |
| 1:B:222:ILE:HG12 | 1:B:246:VAL:HB | 1.98 | 0.43 |
| 1:I:398:TRP:CD1 | 1:I:398:TRP:N | 2.85 | 0.43 |
| 1:I:506:ARG:NH2 | 3:I:940:HOH:O | 2.43 | 0.43 |
| 1:J:142:GLY:HA3 | 1:J:152:ALA:HB3 | 1.99 | 0.43 |
| 3:A:1460:HOH:O | 1:G:102:THR:HG21 | 2.18 | 0.43 |
| 1:H:155:ARG:NH1 | 3:H:915:HOH:O | 2.38 | 0.43 |
| 1:I:334:ASN:HA | 3:I:1003:HOH:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:383:SER:OG | 1:H:384:GLY:N | 2.49 | 0.43 |
| 1:E:108:PRO:HG2 | 1:E:170:VAL:HG11 | 2.00 | 0.43 |
| 1:J:463:SER:HA | 1:J:466:TRP:CE2 | 2.54 | 0.43 |
| 1:C:263:TRP:HB2 | 1:C:364:PRO:HB3 | 2.01 | 0.42 |
| 1:C:365:VAL:HG12 | 1:C:371:PRO:HA | 2.01 | 0.42 |
| 1:E:177:LEU:HD12 | 1:E:422:VAL:HG23 | 2.01 | 0.42 |
| 1:H:584:ARG:NE | 3:H:920:HOH:O | 2.42 | 0.42 |
| 1:J:115:LEU:HD12 | 1:J:159:THR:O | 2.18 | 0.42 |
| 1:E:463:SER:HA | 1:E:466:TRP:CE2 | 2.54 | 0.42 |
| 1:G:127:MET:HE2 | 3:G:1021:HOH:O | 2.17 | 0.42 |
| 1:J:394:TRP:CD1 | 1:J:493:ALA:HB2 | 2.53 | 0.42 |
| 1:A:46:ALA:HA | 1:A:211:PHE:CZ | 2.54 | 0.42 |
| 1:F:399:LEU:C | 1:F:409:ALA:HB2 | 2.40 | 0.42 |
| 1:G:263:TRP:CD2 | 1:G:364:PRO:HA | 2.54 | 0.42 |
| 1:J:339:GLN:HG3 | 1:J:354:VAL:HG21 | 2.01 | 0.42 |
| 1:J:432:PRO:HD2 | 1:J:435:GLN:OE1 | 2.19 | 0.42 |
| 1:A:191:ASP:HA | 1:A:195:ASN:HB3 | 2.00 | 0.42 |
| 1:G:575:PRO:HD3 | 1:G:594:GLU:HG3 | 2.01 | 0.42 |
| 1:I:208:VAL:HG13 | 1:I:212:TYR:HD2 | 1.85 | 0.42 |
| 1:I:53:ALA:HA | 1:I:58:ASN:HB3 | 2.02 | 0.42 |
| 1:J:166:HIS:HE1 | 3:J:972:HOH:O | 2.03 | 0.42 |
| 1:J:444:ASP:O | 1:J:448:ASP:HB2 | 2.19 | 0.42 |
| 1:H:238:PHE:HB3 | 1:H:241:HIS:CD2 | 2.55 | 0.42 |
| 1:J:177:LEU:HD13 | 1:J:418:ARG:HA | 2.00 | 0.42 |
| 1:A:399:LEU:C | 1:A:409:ALA:HB2 | 2.40 | 0.42 |
| 1:I:191:ASP:HA | 1:I:195:ASN:HB3 | 2.01 | 0.42 |
| 1:I:403:ASN:HB3 | 3:I:925:HOH:O | 2.20 | 0.42 |
| 1:J:134:ASN:HB3 | 1:J:163:ASP:O | 2.20 | 0.42 |
| 1:J:189:ARG:NH2 | 3:J:902:HOH:O | 2.49 | 0.42 |
| 1:J:265:THR:HG23 | 1:J:412:VAL:HG12 | 2.01 | 0.42 |
| 1:E:191:ASP:HA | 1:E:195:ASN:HB3 | 2.01 | 0.41 |
| 1:E:248:GLY:HA3 | 1:E:487:TYR:CZ | 2.56 | 0.41 |
| 1:I:336:GLN:NE2 | 3:I:921:HOH:O | 2.25 | 0.41 |
| 1:J:51:CYS:HB2 | 1:J:211:PHE:CE2 | 2.55 | 0.41 |
| 1:J:421:LEU:HD23 | 1:J:421:LEU:HA | 1.95 | 0.41 |
| 1:F:46:ALA:HA | 1:F:211:PHE:CZ | 2.56 | 0.41 |
| 1:F:191:ASP:HA | 1:F:195:ASN:HB3 | 2.01 | 0.41 |
| 1:I:311:ASP:OD1 | 1:I:311:ASP:N | 2.54 | 0.41 |
| 1:J:276:ASP:CG | 1:J:280:VAL:HG22 | 2.41 | 0.41 |
| 1:B:442:LYS:NZ | 3:B:924:HOH:O | 2.49 | 0.41 |
| 1:G:294:LEU:HD11 | 1:G:331:ASN:ND2 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:177:LEU:HD12 | 1:I:422:VAL:HG23 | 2.02 | 0.41 |
| 1:J:421:LEU:HD12 | 1:J:436:VAL:HG13 | 2.02 | 0.41 |
| 1:D:263:TRP:HB2 | 1:D:364:PRO:HB3 | 2.03 | 0.41 |
| 1:G:463:SER:HA | 1:G:466:TRP:CE2 | 2.56 | 0.41 |
| 1:E:263:TRP:CD2 | 1:E:364:PRO:HA | 2.55 | 0.41 |
| 1:H:173:ASN:HB3 | 1:H:176:ALA:HB3 | 2.02 | 0.41 |
| 1:J:239:PRO:HB3 | 3:J:977:HOH:O | 2.20 | 0.41 |
| 1:J:352:VAL:HA | 1:J:355:THR:HG22 | 2.02 | 0.41 |
| 1:B:366:ASN:HB2 | 1:B:446:ASP:OD1 | 2.21 | 0.41 |
| 1:C:191:ASP:HA | 1:C:195:ASN:HB3 | 2.02 | 0.41 |
| 1:E:584:ARG:HD3 | 3:E:1427:HOH:O | 2.21 | 0.41 |
| 1:G:155:ARG:NH1 | 3:G:939:HOH:O | 2.53 | 0.41 |
| 1:G:263:TRP:HB2 | 1:G:364:PRO:HB3 | 2.03 | 0.41 |
| 1:I:208:VAL:HG13 | 1:I:212:TYR:CD2 | 2.56 | 0.41 |
| 1:J:114:ARG:HB2 | 1:J:137:LEU:HD21 | 2.02 | 0.41 |
| 1:B:208:VAL:HG13 | 1:B:212:TYR:HD2 | 1.85 | 0.41 |
| 1:B:263:TRP:CD2 | 1:B:364:PRO:HA | 2.56 | 0.41 |
| 1:J:280:VAL:HG21 | 1:J:437:ALA:HB1 | 2.03 | 0.41 |
| 1:A:248:GLY:HA3 | 1:A:487:TYR:CZ | 2.56 | 0.40 |
| 1:F:43:VAL:HA | 1:F:44:PRO:HD3 | 1.94 | 0.40 |
| 1:F:254:LEU:CD2 | 1:F:495:PHE:CE1 | 3.04 | 0.40 |
| 1:H:399:LEU:C | 1:H:409:ALA:HB2 | 2.41 | 0.40 |
| 1:A:263:TRP:HB2 | 1:A:364:PRO:HB3 | 2.03 | 0.40 |
| 1:B:191:ASP:HA | 1:B:195:ASN:HB3 | 2.02 | 0.40 |
| 1:C:379:ASP:OD2 | 1:C:491:SER:OG | 2.34 | 0.40 |
| 1:H:317:TYR:CZ | 1:H:522:LEU:HD12 | 2.56 | 0.40 |
| 1:F:317:TYR:O | 1:F:321:GLN:HG2 | 2.22 | 0.40 |
| 1:H:365:VAL:HG12 | 1:H:371:PRO:HA | 2.04 | 0.40 |
| 1:J:350:SER:HB2 | 1:J:353:GLN:H | 1.87 | 0.40 |
| 1:J:208:VAL:HG22 | 3:J:1108:HOH:O | 2.21 | 0.40 |
| 1:J:243:ASP:O | 1:J:482:GLY:HA2 | 2.21 | 0.40 |
| 1:J:484:MET:SD | 1:J:486:LEU:HD21 | 2.62 | 0.40 |
| 1:D:399:LEU:C | 1:D:409:ALA:HB2 | 2.41 | 0.40 |

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:1449:HOH:O | 3:H:1218:HOH:O[1_655] | 1.83 | 0.37 |
| 3:D:1450:HOH:O | 3:E:1566:HOH:O[1_455] | 1.92 | 0.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:1307:HOH:O | 3:G:1262:HOH:O[1_655] | 1.93 | 0.27 |
| 3:A:1530:HOH:O | 3:G:1310:HOH:O[1_655] | 2.01 | 0.19 |
| 3:D:1176:HOH:O | 3:E:1039:HOH:O[1_455] | 2.02 | 0.18 |
| 3:E:1548:HOH:O | 3:H:1292:HOH:O[1_655] | 2.02 | 0.18 |
| 3:C:1669:HOH:O | 3:D:1586:HOH:O[1_645] | 2.05 | 0.15 |
| 3:C:1188:HOH:O | 3:E:1226:HOH:O[1_545] | 2.06 | 0.14 |
| 3:B:1369:HOH:O | 3:F:1518:HOH:O[1_556] | 2.08 | 0.12 |
| 3:E:1591:HOH:O | 3:H:1342:HOH:O[1_655] | 2.09 | 0.11 |
| 3:E:904:HOH:O | 3:J:1039:HOH:O[1_655] | 2.13 | 0.07 |
| 3:C:1261:HOH:O | 3:E:1262:HOH:O[1_545] | 2.18 | 0.02 |
| 3:A:1307:HOH:O | 3:G:1372:HOH:O[1_655] | 2.19 | 0.01 |
| 3:A:1480:HOH:O | 3:G:1347:HOH:O[1_655] | 2.19 | 0.01 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 560/611 (92%) | 544 (97%) | 16 (3%) | 0 | 100 | 100 |
| 1 | B | 559/611 (92%) | 543 (97%) | 16 (3%) | 0 | 100 | 100 |
| 1 | C | 559/611 (92%) | 544 (97%) | 15 (3%) | 0 | 100 | 100 |
| 1 | D | 559/611 (92%) | 541 (97%) | 18 (3%) | 0 | 100 | 100 |
| 1 | E | 559/611 (92%) | 545 (98%) | 14 (2%) | 0 | 100 | 100 |
| 1 | F | 559/611 (92%) | 544 (97%) | 15 (3%) | 0 | 100 | 100 |
| 1 | G | 560/611 (92%) | 547 (98%) | 13 (2%) | 0 | 100 | 100 |
| 1 | H | 560/611 (92%) | 544 (97%) | 16 (3%) | 0 | 100 | 100 |
| 1 | I | 559/611 (92%) | 540 (97%) | 19 (3%) | 0 | 100 | 100 |
| 1 | J | 558/611 (91%) | 536 (96%) | 21 (4%) | 1 (0%) | 47 | 38 |
| All | All | 5592/6110 (92%) | 5428 (97%) | 163 (3%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 50 | ALA |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 408/449 (91%) | 405 (99%) | 3 (1%) | 84 | 84 |
| 1 | B | 407/449 (91%) | 406 (100%) | 1 (0%) | 93 | 94 |
| 1 | C | 407/449 (91%) | 403 (99%) | 4 (1%) | 76 | 76 |
| 1 | D | 407/449 (91%) | 405 (100%) | 2 (0%) | 88 | 89 |
| 1 | E | 407/449 (91%) | 404 (99%) | 3 (1%) | 84 | 84 |
| 1 | F | 407/449 (91%) | 404 (99%) | 3 (1%) | 84 | 84 |
| 1 | G | 408/449 (91%) | 405 (99%) | 3 (1%) | 84 | 84 |
| 1 | H | 408/449 (91%) | 404 (99%) | 4 (1%) | 76 | 76 |
| 1 | I | 407/449 (91%) | 405 (100%) | 2 (0%) | 88 | 89 |
| 1 | J | 406/449 (90%) | 398 (98%) | 8 (2%) | 55 | 51 |
| All | All | 4072/4490 (91%) | 4039 (99%) | 33 (1%) | 81 | 82 |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 241 | HIS |
| 1 | A | 375 | ARG |
| 1 | A | 538 | PHE |
| 1 | B | 375 | ARG |
| 1 | C | 48 | ARG |
| 1 | C | 241 | HIS |
| 1 | C | 375 | ARG |
| 1 | C | 433 | MET |
| 1 | D | 241 | HIS |
| 1 | D | 375 | ARG |
| 1 | E | 241 | HIS |
| 1 | E | 375 | ARG |
| 1 | E | 538 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 210 | ARG |
| 1 | F | 241 | HIS |
| 1 | F | 375 | ARG |
| 1 | G | 241 | HIS |
| 1 | G | 375 | ARG |
| 1 | G | 538 | PHE |
| 1 | H | 240 | SER |
| 1 | H | 375 | ARG |
| 1 | H | 538 | PHE |
| 1 | H | 550 | ARG |
| 1 | I | 358 | LYS |
| 1 | I | 375 | ARG |
| 1 | J | 60 | ASP |
| 1 | J | 112 | LYS |
| 1 | J | 163 | ASP |
| 1 | J | 210 | ARG |
| 1 | J | 211 | PHE |
| 1 | J | 352 | VAL |
| 1 | J | 375 | ARG |
| 1 | J | 538 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 403 | ASN |
| 1 | J | 241 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 562/611 (91%) | -0.09 | 6 (1%) | 80 | 82 | 13, 20, 33, 63 | 0 |
| 1 | B | 561/611 (91%) | 0.00 | 4 (0%) | 87 | 88 | 12, 19, 31, 57 | 0 |
| 1 | C | 561/611 (91%) | -0.11 | 5 (0%) | 84 | 85 | 11, 19, 31, 53 | 0 |
| 1 | D | 561/611 (91%) | -0.03 | 4 (0%) | 87 | 88 | 14, 21, 33, 61 | 0 |
| 1 | E | 561/611 (91%) | 0.04 | 3 (0%) | 91 | 92 | 14, 21, 33, 59 | 0 |
| 1 | F | 561/611 (91%) | -0.16 | 4 (0%) | 87 | 88 | 11, 20, 33, 57 | 0 |
| 1 | G | 562/611 (91%) | -0.11 | 4 (0%) | 87 | 88 | 18, 27, 38, 66 | 0 |
| 1 | H | 562/611 (91%) | 0.35 | 22 (3%) | 39 | 42 | 21, 31, 50, 70 | 0 |
| 1 | I | 561/611 (91%) | 0.98 | 95 (16%) | 1 | 1 | 26, 41, 59, 72 | 0 |
| 1 | J | 560/611 (91%) | 1.25 | 136 (24%) | 0 | 0 | 28, 49, 64, 80 | 0 |
| All | All | 5612/6110 (91%) | 0.21 | 283 (5%) | 28 | 32 | 11, 24, 54, 80 | 0 |

All (283) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 43 | VAL | 7.3 |
| 1 | E | 57 | GLY | 6.9 |
| 1 | I | 603 | PRO | 6.8 |
| 1 | J | 63 | TRP | 6.3 |
| 1 | I | 602 | PRO | 6.2 |
| 1 | J | 177 | LEU | 5.9 |
| 1 | I | 585 | TYR | 5.6 |
| 1 | I | 584 | ARG | 5.3 |
| 1 | F | 57 | GLY | 5.2 |
| 1 | J | 184 | LEU | 5.2 |
| 1 | H | 57 | GLY | 5.1 |
| 1 | J | 514 | ALA | 5.0 |
| 1 | I | 341 | VAL | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | I | 308 | GLY | 5.0 |
| 1 | A | 42 | PRO | 4.8 |
| 1 | J | 164 | GLY | 4.8 |
| 1 | C | 57 | GLY | 4.7 |
| 1 | B | 57 | GLY | 4.7 |
| 1 | C | 58 | ASN | 4.6 |
| 1 | H | 45 | LEU | 4.6 |
| 1 | I | 600 | ALA | 4.5 |
| 1 | J | 43 | VAL | 4.4 |
| 1 | F | 58 | ASN | 4.4 |
| 1 | J | 57 | GLY | 4.3 |
| 1 | I | 598 | ALA | 4.3 |
| 1 | J | 169 | ALA | 4.3 |
| 1 | H | 44 | PRO | 4.2 |
| 1 | I | 305 | ALA | 4.2 |
| 1 | I | 512 | PRO | 4.2 |
| 1 | J | 188 | ALA | 4.1 |
| 1 | J | 600 | ALA | 4.1 |
| 1 | H | 368 | ALA | 4.1 |
| 1 | J | 369 | GLY | 4.1 |
| 1 | J | 51 | CYS | 4.0 |
| 1 | I | 309 | LEU | 4.0 |
| 1 | J | 102 | THR | 4.0 |
| 1 | J | 69 | VAL | 4.0 |
| 1 | I | 380 | ALA | 4.0 |
| 1 | I | 457 | GLY | 3.9 |
| 1 | I | 514 | ALA | 3.9 |
| 1 | D | 57 | GLY | 3.9 |
| 1 | J | 447 | ILE | 3.8 |
| 1 | J | 211 | PHE | 3.8 |
| 1 | J | 457 | GLY | 3.8 |
| 1 | J | 412 | VAL | 3.8 |
| 1 | F | 56 | ASP | 3.8 |
| 1 | J | 56 | ASP | 3.7 |
| 1 | J | 459 | PHE | 3.6 |
| 1 | J | 109 | TYR | 3.6 |
| 1 | I | 583 | ALA | 3.6 |
| 1 | J | 62 | VAL | 3.6 |
| 1 | I | 377 | ALA | 3.5 |
| 1 | G | 58 | ASN | 3.5 |
| 1 | J | 584 | ARG | 3.5 |
| 1 | I | 529 | CYS | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 42 | PRO | 3.5 |
| 1 | J | 279 | GLY | 3.5 |
| 1 | I | 588 | SER | 3.5 |
| 1 | J | 422 | VAL | 3.4 |
| 1 | J | 403 | ASN | 3.4 |
| 1 | I | 313 | ILE | 3.4 |
| 1 | I | 340 | CYS | 3.4 |
| 1 | J | 341 | VAL | 3.4 |
| 1 | H | 208 | VAL | 3.3 |
| 1 | I | 312 | GLY | 3.3 |
| 1 | I | 550 | ARG | 3.3 |
| 1 | J | 417 | ALA | 3.3 |
| 1 | J | 482 | GLY | 3.3 |
| 1 | J | 598 | ALA | 3.3 |
| 1 | I | 336 | GLN | 3.3 |
| 1 | J | 241 | HIS | 3.3 |
| 1 | J | 458 | GLN | 3.3 |
| 1 | J | 104 | ILE | 3.3 |
| 1 | I | 454 | ALA | 3.3 |
| 1 | J | 415 | PHE | 3.2 |
| 1 | J | 106 | GLY | 3.2 |
| 1 | J | 180 | VAL | 3.2 |
| 1 | J | 481 | GLY | 3.2 |
| 1 | J | 176 | ALA | 3.2 |
| 1 | I | 294 | LEU | 3.1 |
| 1 | A | 57 | GLY | 3.1 |
| 1 | C | 59 | GLY | 3.1 |
| 1 | I | 548 | VAL | 3.1 |
| 1 | I | 515 | ALA | 3.1 |
| 1 | J | 551 | GLY | 3.1 |
| 1 | I | 510 | ALA | 3.0 |
| 1 | I | 553 | ALA | 3.0 |
| 1 | I | 369 | GLY | 3.0 |
| 1 | I | 310 | ALA | 3.0 |
| 1 | I | 329 | ALA | 3.0 |
| 1 | I | 306 | LEU | 3.0 |
| 1 | J | 58 | ASN | 3.0 |
| 1 | J | 107 | TYR | 3.0 |
| 1 | I | 567 | PHE | 2.9 |
| 1 | C | 60 | ASP | 2.9 |
| 1 | J | 44 | PRO | 2.9 |
| 1 | I | 599 | CYS | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | I | 474 | LEU | 2.9 |
| 1 | J | 474 | LEU | 2.9 |
| 1 | J | 477 | PHE | 2.9 |
| 1 | J | 466 | TRP | 2.9 |
| 1 | J | 200 | VAL | 2.9 |
| 1 | J | 61 | MET | 2.9 |
| 1 | J | 437 | ALA | 2.9 |
| 1 | I | 556 | GLN | 2.9 |
| 1 | I | 587 | GLY | 2.9 |
| 1 | I | 522 | LEU | 2.9 |
| 1 | A | 60 | ASP | 2.9 |
| 1 | J | 105 | ASP | 2.9 |
| 1 | J | 203 | ALA | 2.9 |
| 1 | J | 450 | LEU | 2.8 |
| 1 | J | 66 | ALA | 2.8 |
| 1 | J | 101 | ARG | 2.8 |
| 1 | I | 486 | LEU | 2.8 |
| 1 | J | 121 | TRP | 2.8 |
| 1 | J | 190 | LEU | 2.8 |
| 1 | I | 601 | ALA | 2.8 |
| 1 | B | 59 | GLY | 2.8 |
| 1 | H | 56 | ASP | 2.8 |
| 1 | I | 568 | GLY | 2.8 |
| 1 | D | 59 | GLY | 2.8 |
| 1 | G | 57 | GLY | 2.8 |
| 1 | I | 482 | GLY | 2.8 |
| 1 | I | 348 | CYS | 2.8 |
| 1 | H | 49 | ALA | 2.7 |
| 1 | C | 56 | ASP | 2.7 |
| 1 | I | 367 | SER | 2.7 |
| 1 | J | 181 | ALA | 2.7 |
| 1 | I | 333 | ALA | 2.7 |
| 1 | J | 65 | ASN | 2.7 |
| 1 | J | 275 | LEU | 2.7 |
| 1 | I | 509 | ALA | 2.7 |
| 1 | J | 70 | VAL | 2.7 |
| 1 | J | 54 | LEU | 2.7 |
| 1 | I | 594 | GLU | 2.7 |
| 1 | H | 481 | GLY | 2.7 |
| 1 | J | 454 | ALA | 2.6 |
| 1 | I | 575 | PRO | 2.6 |
| 1 | H | 58 | ASN | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 442 | LYS | 2.6 |
| 1 | J | 175 | ASP | 2.6 |
| 1 | J | 108 | PRO | 2.6 |
| 1 | J | 602 | PRO | 2.6 |
| 1 | J | 170 | VAL | 2.6 |
| 1 | J | 206 | ALA | 2.6 |
| 1 | E | 56 | ASP | 2.6 |
| 1 | J | 427 | PRO | 2.6 |
| 1 | J | 179 | THR | 2.6 |
| 1 | E | 58 | ASN | 2.6 |
| 1 | J | 195 | ASN | 2.6 |
| 1 | J | 421 | LEU | 2.6 |
| 1 | J | 515 | ALA | 2.6 |
| 1 | I | 547 | TRP | 2.6 |
| 1 | J | 462 | SER | 2.6 |
| 1 | J | 98 | ILE | 2.6 |
| 1 | H | 47 | SER | 2.5 |
| 1 | A | 56 | ASP | 2.5 |
| 1 | J | 208 | VAL | 2.5 |
| 1 | I | 517 | PHE | 2.5 |
| 1 | J | 216 | ALA | 2.5 |
| 1 | J | 242 | TYR | 2.5 |
| 1 | J | 330 | ALA | 2.5 |
| 1 | J | 373 | TYR | 2.5 |
| 1 | H | 552 | GLU | 2.5 |
| 1 | I | 347 | ASP | 2.5 |
| 1 | I | 303 | CYS | 2.5 |
| 1 | I | 555 | ASP | 2.5 |
| 1 | I | 592 | ASN | 2.5 |
| 1 | J | 465 | ASP | 2.5 |
| 1 | I | 576 | LEU | 2.5 |
| 1 | J | 306 | LEU | 2.5 |
| 1 | J | 136 | SER | 2.5 |
| 1 | J | 376 | TRP | 2.5 |
| 1 | I | 323 | ALA | 2.5 |
| 1 | J | 96 | GLY | 2.5 |
| 1 | J | 434 | THR | 2.5 |
| 1 | B | 56 | ASP | 2.5 |
| 1 | J | 319 | ALA | 2.5 |
| 1 | J | 273 | VAL | 2.5 |
| 1 | I | 324 | PHE | 2.5 |
| 1 | J | 455 | THR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 435 | GLN | 2.4 |
| 1 | J | 277 | ALA | 2.4 |
| 1 | I | 574 | ARG | 2.4 |
| 1 | J | 599 | CYS | 2.4 |
| 1 | H | 216 | ALA | 2.4 |
| 1 | J | 310 | ALA | 2.4 |
| 1 | A | 58 | ASN | 2.4 |
| 1 | J | 48 | ARG | 2.4 |
| 1 | I | 586 | LYS | 2.4 |
| 1 | I | 334 | ASN | 2.4 |
| 1 | I | 511 | MET | 2.4 |
| 1 | I | 292 | LEU | 2.4 |
| 1 | I | 346 | ALA | 2.4 |
| 1 | J | 333 | ALA | 2.4 |
| 1 | J | 60 | ASP | 2.4 |
| 1 | I | 569 | VAL | 2.4 |
| 1 | F | 60 | ASP | 2.4 |
| 1 | J | 67 | ALA | 2.4 |
| 1 | H | 455 | THR | 2.4 |
| 1 | J | 178 | GLY | 2.4 |
| 1 | J | 512 | PRO | 2.4 |
| 1 | I | 290 | ALA | 2.3 |
| 1 | J | 252 | TYR | 2.3 |
| 1 | J | 509 | ALA | 2.3 |
| 1 | B | 58 | ASN | 2.3 |
| 1 | I | 297 | GLN | 2.3 |
| 1 | D | 58 | ASN | 2.3 |
| 1 | I | 242 | TYR | 2.3 |
| 1 | J | 479 | ASP | 2.3 |
| 1 | J | 420 | TRP | 2.3 |
| 1 | J | 135 | GLY | 2.3 |
| 1 | J | 432 | PRO | 2.3 |
| 1 | I | 507 | LEU | 2.3 |
| 1 | J | 280 | VAL | 2.3 |
| 1 | G | 602 | PRO | 2.3 |
| 1 | I | 447 | ILE | 2.3 |
| 1 | J | 601 | ALA | 2.3 |
| 1 | I | 477 | PHE | 2.2 |
| 1 | J | 113 | PHE | 2.2 |
| 1 | J | 192 | MET | 2.2 |
| 1 | I | 316 | ASN | 2.2 |
| 1 | J | 74 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 100 | LYS | 2.2 |
| 1 | J | 486 | LEU | 2.2 |
| 1 | I | 481 | GLY | 2.2 |
| 1 | I | 505 | GLU | 2.2 |
| 1 | H | 217 | ASP | 2.2 |
| 1 | I | 330 | ALA | 2.2 |
| 1 | I | 520 | LEU | 2.2 |
| 1 | I | 370 | THR | 2.2 |
| 1 | I | 475 | ALA | 2.2 |
| 1 | J | 182 | PHE | 2.2 |
| 1 | J | 577 | CYS | 2.2 |
| 1 | J | 232 | MET | 2.2 |
| 1 | J | 68 | THR | 2.2 |
| 1 | I | 487 | TYR | 2.2 |
| 1 | J | 508 | GLY | 2.2 |
| 1 | J | 221 | PHE | 2.2 |
| 1 | H | 474 | LEU | 2.1 |
| 1 | J | 133 | THR | 2.1 |
| 1 | J | 460 | THR | 2.1 |
| 1 | I | 343 | ALA | 2.1 |
| 1 | J | 453 | TRP | 2.1 |
| 1 | I | 390 | TYR | 2.1 |
| 1 | J | 212 | TYR | 2.1 |
| 1 | H | 548 | VAL | 2.1 |
| 1 | J | 52 | GLU | 2.1 |
| 1 | I | 132 | GLY | 2.1 |
| 1 | I | 532 | GLY | 2.1 |
| 1 | H | 365 | VAL | 2.1 |
| 1 | J | 441 | MET | 2.1 |
| 1 | I | 577 | CYS | 2.1 |
| 1 | H | 78 | ALA | 2.1 |
| 1 | I | 216 | ALA | 2.1 |
| 1 | I | 544 | LEU | 2.1 |
| 1 | J | 425 | ALA | 2.1 |
| 1 | J | 579 | TYR | 2.1 |
| 1 | J | 251 | GLY | 2.1 |
| 1 | J | 233 | MET | 2.1 |
| 1 | J | 445 | PHE | 2.1 |
| 1 | J | 245 | ILE | 2.1 |
| 1 | J | 404 | SER | 2.1 |
| 1 | J | 172 | ASP | 2.1 |
| 1 | A | 59 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | I | 546 | ALA | 2.1 |
| 1 | J | 168 | ASN | 2.1 |
| 1 | I | 554 | PRO | 2.1 |
| 1 | I | 252 | TYR | 2.0 |
| 1 | J | 424 | PHE | 2.0 |
| 1 | H | 118 | PRO | 2.0 |
| 1 | H | 213 | GLY | 2.0 |
| 1 | J | 568 | GLY | 2.0 |
| 1 | J | 520 | LEU | 2.0 |
| 1 | D | 60 | ASP | 2.0 |
| 1 | I | 479 | ASP | 2.0 |
| 1 | I | 472 | THR | 2.0 |
| 1 | I | 526 | MET | 2.0 |
| 1 | G | 56 | ASP | 2.0 |
| 1 | I | 590 | ASP | 2.0 |
| 1 | I | 498 | LEU | 2.0 |
| 1 | I | 328 | THR | 2.0 |
| 1 | J | 471 | SER | 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 monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | CA | I | 801 | 1/1 | 0.91 | 0.07 | 47,47,47,47 | 0 |
| 2 | CA | B | 801 | 1/1 | 0.97 | 0.37 | 51,51,51,51 | 0 |
| 2 | CA | J | 801 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 2 | CA | F | 801 | 1/1 | 0.99 | 0.11 | 23,23,23,23 | 0 |
| 2 | CA | G | 801 | 1/1 | 0.99 | 0.08 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | CA | H | 801 | 1/1 | 0.99 | 0.09 | 26,26,26,26 | 0 |
| 2 | CA | A | 801 | 1/1 | 0.99 | 0.12 | 21,21,21,21 | 0 |
| 2 | CA | C | 801 | 1/1 | 0.99 | 0.08 | 19,19,19,19 | 0 |
| 2 | CA | E | 801 | 1/1 | 1.00 | 0.10 | 21,21,21,21 | 0 |
| 2 | CA | D | 801 | 1/1 | 1.00 | 0.15 | 20,20,20,20 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.