Data collection and refinement statistics for project **mes_3k4l** crystal **crystal1**

model: `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3k4l/structure_mr/build_model_3/hkl_import.pdb_tls` vs model: `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3k4l/structure_mr/build_model_3/hkl_refine_42.pdb`

### Data collection

|                          | 3K4L                      | Re-refinement          |
|--------------------------|---------------------------|------------------------|
| Resolution (Å)           | 30.00 - 1.75 (1.80 - 1.75)| 28.66 - 1.75           |
| Wavelength (Å)           | 1.0379                    |                        |
| Space group              | P43212                    | P43212                 |
| a, b, c (Å)              | 101.57, 101.57, 250.05    | 101.57, 101.57, 250.05 |
| α, β, γ (°)              | 90, 90, 90                | 90, 90, 90             |
| Completeness (%)         | 99.9 (99.9)               | 99.9 (99.9)            |
| Reflections used         | 132005                    |                        |
| <I> / <Sigma I>          | 15.4 (2.5)                |                        |
| Redundancy               | 7.3 (7.3)                 |                        |
| Rmerge                   | 0.102 (0.883)             |                        |
| Wilson B factor (Å²)     | 17.3                      |                        |

### Refinement

|                          | 3K4L                      | Re-refinement          |
|--------------------------|---------------------------|------------------------|
| Rwork / Rfree            | 0.175 / 0.209             | 0.178 / 0.210          |
| Resolution (Å)           | 30.00 - 1.75              | 28.66 - 1.75           |
| Reflections all          | 130031                    | 132005                 |
| Reflections for Rfree    | 1974, 1.5%                | 1974, 1.5%             |
| Bond lengths rmsd (Å)    | 0.021                     | 0.025                  |
| Bond angles rmsd (°)     | 1.99                      | 2.29                   |
| Mean B value (Å²)        | 20                        | 19                     |
| Number of protein atoms  | 8944                      | 8944                   |
| Mean B value for protein atoms (Å²) | 20 | 19 |
| Number of water atoms (expected) | 722 (1322) | 722 (1322) |
| Mean B value for water atoms (Å²) | 25 | 23 |
| Number of ligand/ion atoms | 166 | 166 |
| Mean B value for ligand/ion atoms (Å²) | 20 | 19 |
| Clashscore               | 3.92                      | 3.86                   |
| Clashscore percentile (100) | -1                       | -1                     |
| Rotamer outliers (<1%)   | 1.21                      | 1.21                   |
| Ramachandran outliers (<0.2%) | 0.00                 | 0.00                   |
| Ramachandran favored (>98%) | 97.25                  | 97.25                  |
| Residues with bad bonds (<0%) | 2.38                  | 2.47                   |
| Residues with bad angles (<0%) | 4.50                  | 4.32                   |
| MolProbity score         | 1.38                      | 1.38                   |

**Map cc barchart:**
Small molecules with map:
Small molecule 1: FLAVIN-ADENINE DINUCLEOTIDE (FAD) A 801 map cc 0.99

Small molecule 2: 2-deoxy-2-fluoro-beta-D-glucopyranos (SHG) A 901 map cc 0.93

Small molecule 3: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 902 map cc 0.93

Small molecule 4: FLAVIN-ADENINE DINUCLEOTIDE (FAD) B 801 map cc 0.98
Small molecule 5: 2-deoxy-2-fluoro-beta-D-glucopyranos (SHG) B 901 map cc 0.92

Small molecule 6: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 903 map cc 0.98

Small molecule 7: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 902 map cc 0.91

Credits:
HKL-3000
"Processing of X-ray Diffraction Data Collected in Oscillation Mode"
Z. Otwinowski, W. Minor
Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p307-326 (1997)

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Reffmac5
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Data collection and refinement statistics for project **mes_3k4l crystal crystal1**

Model `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3k4l/structure_mr/build_model_3/hkl_import.pdb_tls` vs model `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3k4l/structure_mr/build_model_3/hkl_refine_40.pdb_tls`

| Data collection | 3K4L | Re-refinement |
|-----------------|------|--------------|
| Resolution (Å)  | 30.00 - 1.75 (1.80 - 1.75) | 28.66 - 1.75 |
| Wavelength (Å)  | 1.0379 | |
| Space group     | P43212 | P43212 |
| a, b, c (Å)     | 101.57, 101.57, 250.05 | 101.57, 101.57, 250.05 |
| α, β, γ (°)     | 90, 90, 90 | 90, 90, 90 |
| Completeness (%)| 99.9 (99.9) | 99.9 (99.9) |
| Reflections used| 132005 | |
| <I>/ <Sigma I> | 15.4 (2.5) | |
| Redundancy      | 7.3 (7.3) | |
| Rmerge          | 0.102 (0.883) | |
| Wilson B factor (Å²) | 17.3 | |

| Refinement | 3K4L | Re-refinement |
|------------|------|--------------|
| Rwork / Rfree | 0.175 / 0.209 | 0.173 / 0.201 |
| Resolution (Å) | 30.00 - 1.75 | 28.66 - 1.75 |
| Reflections all | 130031 | 132005 |
| Reflections for Rfree | 1974, 1.5% | 1974, 1.5% |
| Bond lengths rmsd (Å) | 0.021 | 0.015 |
| Bond angles rmsd (°) | 1.99 | 1.92 |
| Mean B value (Å²) | 20 | 20 |
| Number of protein atoms | 8944 | 8988 |
| Mean B value for protein atoms (Å²) | 20 | 19 |
| Number of water atoms (expected) | 722 (1322) | 729 (1322) |
| Mean B value for water atoms (Å²) | 25 | 23 |
| Number of ligand/ion atoms | 166 | 166 |
| Mean B value for ligand/ion atoms (Å²) | 20 | 19 |
| Clashscore | 3.92 | 2.00 |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 1.21 | 0.70 |
| Ramachandran outliers (<0.2%) | 0.00 | 0.00 |
| Ramachandran favored (>98%) | 97.25 | 97.87 |
| Residues with bad bonds (<0%) | 2.38 | 1.14 |
| Residues with bad angles (<0.1%) | 4.50 | 2.64 |
| MolProbity score | 1.38 | 1.00 |

Map cc barchart:
Small molecules with map:
Small molecule 1: FLAVIN-ADENINE DINUCLEOTIDE (FAD) A 801 map cc 0.98

Small molecule 2: 2-deoxy-2-fluoro-beta-D-glucopyranos (SHG) A 901 map cc 0.94

Small molecule 3: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 902 map cc 0.94

Small molecule 4: FLAVIN-ADENINE DINUCLEOTIDE (FAD) B 801 map cc 0.98
Small molecule 5: 2-deoxy-2-fluoro-beta-D-glucopyranos (SHG) B 901 map cc 0.93

Small molecule 6: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 902 map cc 0.92

Small molecule 7: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 903 map cc 0.99

Credits:
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Data collection and refinement statistics for project **mes_3pyi** crystal **crystal1**

```plaintext
model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3pyi/structure_mr/build_model_2/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3pyi/structure_mr/build_model_2/hkl_refine_45.pdb
```

| **Data collection** | 3PYI | Re-refinement |
|---------------------|------|---------------|
| Resolution (Å)      | 73.15 - 2.10 (2.22 - 2.10) | 50.68 - 2.10 |
| Wavelength (Å)      | 1.0  |               |
| Space group         | P212121 | P212121        |
| a, b, c (Å)         | 70.27, 73.15, 79.60 | 70.27, 73.15, 79.60 |
| α, β, γ (*)         | 90, 90, 90 | 90, 90, 90     |
| Completeness (%)    | 99.6 (99.3) | 100.0 (100.0) |
| Reflected used      | 24368 |               |
| <I>/<<Sigma I>      | 17.7 (4.0) |               |
| Redundancy          | 3.6 (3.6) |               |
| Rmerge              | 0.039 |               |
| Rpm                 |      |               |
| CC1/2 last shell    |      |               |
| Wilson B factor (Å²)| 31.5 |               |

| **Refinement**      |       |               |
|---------------------|------|---------------|
| Rwork / Rfree       | 0.210 / 0.257 | 0.222 / 0.259 |
| Resolution (Å)      | 50.68 - 2.10 | 50.69 - 2.10  |
| Reflections all     | 23106 | 24319         |
| Reflections for Rfree | 2220, 4.9% | 1213, 5.0%   |
| Bond lengths rmsd (Å) | 0.007 | 0.015         |
| Bond angles rmsd (°)| 1.02  | 1.75          |
| Mean B value (Å²)   | 46    | 44            |
| Number of protein atoms | 2352 | 2352          |
| Mean B value for protein atoms (Å²) | 45 | 42 |
| Number of water atoms (expected) | 146 (263) | 146 (263) |
| Mean B value for water atoms (Å²) | 46 | 48 |
| Number of ligand/ion atoms | 49 | 49 |
| Mean B value for ligand/ion atoms (Å²) | 94 | 88 |
| Clashscore          | 5.93  | 5.92          |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 0.00 | 0.00 |
| Ramachandran outliers (<0.2%) | 0.36 | 0.36 |
| Ramachandran favored (>98%) | 98.19 | 98.19 |
| Residues with bad bonds (<0%) | 0.00 | 0.18 |
| Residues with bad angles (<0.1%) | 0.00 | 0.00 |
| MolProbity score    | 1.32  | 1.32          |

**Map cc bar chart:**
Small molecules with map:

Small molecule 1: TETRAETHYLENE GLYCOL (PG4) B 169 map cc 0.76

Small molecule 2: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 170 map cc 0.54
Small molecule 3: TETRAETHYLENE GLYCOL (PG4) B 171 map cc 0.54

Small molecule 4: TETRAETHYLENE GLYCOL (PG4) A 169 map cc 0.88

Small molecule 5: TETRAETHYLENE GLYCOL (PG4) A 170 map cc 0.51

Credits:
HKL-3000
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Coot
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Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **mes_3pyi crystal crystal1**

|                  | 3PYI                              | Re-refinement                  |
|------------------|-----------------------------------|--------------------------------|
| Resolution (Å)   | 73.15 - 2.10 (2.22 - 2.10)        | 50.68 - 2.10                   |
| Wavelength (Å)   | 1.0                               |                                |
| Space group      | P212121                           | P212121                        |
| a, b, c (Å)      | 70.27, 73.15, 79.60               | 70.27, 73.15, 79.60            |
| α, β, γ (°)      | 90, 90, 90                        | 90, 90, 90                     |
| Completeness (%) | 99.6 (99.3)                       | 100.0 (100.0)                  |
| Reflections used | 24368                             |                                |
| <I> / <Sigma I> | 17.7 (4.0)                        |                                |
| Redundancy       | 3.6 (3.6)                         |                                |
| Rmerge           | 0.039                             |                                |
| Rpim             |                                   |                                |
| Wilson B factor (Å²) |                              | 31.5                           |

**Refinement**

|                  | 0.210 / 0.257                     | 0.205 / 0.262                  |
| Resolution (Å)   | 50.68 - 2.10                      | 50.69 - 2.10                   |
| Reflections all  | 23106                             | 24319                          |
| Reflections for Rfree | 2220, 4.9%                  | 1213, 5.0%                     |
| Bond lengths rmsd (Å) | 0.007                          | 0.014                          |
| Bond angles rmsd (°) | 1.02                           | 1.91                           |
| Mean B value (Å²) | 46                               | 44                             |
| Number of protein atoms | 2352                           | 2340                           |
| Mean B value for protein atoms (Å²) | 45                         | 43                             |
| Number of water atoms (expected) | 146 (263)                      | 133 (263)                      |
| Mean B value for water atoms (Å²) | 46                           | 47                             |
| Number of ligand/ion atoms | 49                            | 51                             |
| Mean B value for ligand/ion atoms (Å²) | 94                          | 90                             |
| Clashscore       | 5.93                             | 2.47                           |
| Clashscore percentile (100) | -1                        | -1                             |
| Rotamer outliers (<1%) | 0.00                       | 0.37                           |
| Ramachandran outliers (<0.2%) | 0.36                       | 0.00                           |
| Ramachandran favored (>98%) | 98.19                      | 98.19                          |
| Residues with bad bonds (<0%) | 0.00                        | 0.88                           |
| Residues with bad angles (<0.1%) | 0.00                      | 2.63                           |
| MolProbity score | 1.32                             | 1.03                           |

Map cc barchart:
Small molecules with map:

Small molecule 1: TETRAETHYLENE GLYCOL (PG4) A 169 map cc 0.85

Small molecule 2: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 170 map cc 0.77
Small molecule 3: TETRAETHYLENE GLYCOL (PG4) B 169 map cc 0.82

Small molecule 4: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 170 map cc 0.61

Small molecule 5: TETRAETHYLENE GLYCOL (PG4) B 171 map cc 0.87

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Data collection and refinement statistics for project **hepes_5t6l crystal crystal1**

Model `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3t6l/structure_mr/build_model_2/hkl_import.pdb` vs model `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/3t6l/structure_mr/build_model_2/hkl_refine_38.pdb`

### Data collection

| Feature                        | 5T6L                              | Re-refinement                      |
|--------------------------------|-----------------------------------|------------------------------------|
| Resolution (Å)                 | 47.14 - 2.10 (2.15 - 2.10)        | 47.14 - 2.10                       |
| Wavelength (Å)                 | 1.03314                           |                                    |
| Space group                    | P21                               | P21                                |
| a, b, c (Å)                    | 41.10, 158.97, 99.69               | 41.10, 158.97, 99.69               |
| α, β, γ (°)                    | 90, 97.98, 90                      | 90, 97.98, 90                      |
| Completeness (%)               | 97.5 (91.9)                        | 100.0 (100.0)                      |
| Reflections used               | 72210                             |                                    |
| <I> / <Sigma I>                | 9.3 (1.6)                          |                                    |
| Redundancy                     | 2.4 (2.3)                          |                                    |
| Rmerge                         | 0.074                             |                                    |
| Wilson B factor (Å²)           |                                     |                                    |
| CC1/2 last shell               |                                    |                                    |
| Wilson B factor (Å²)           | 31.3                               |                                    |

### Refinement

| Feature                        | 5T6L                              | Re-refinement                      |
|--------------------------------|-----------------------------------|------------------------------------|
| Rwork / Rfree                  | 0.178 / 0.218                     | 0.197 / 0.230                      |
| Resolution (Å)                 | 47.14 - 2.10                      | 47.14 - 2.10                       |
| Reflections all                | 72183                             | 72118                              |
| Reflections for Rfree          | 3620.50%                          | 3615.50%                           |
| Bond lengths rmsd (Å)          | 0.008                             | 0.015                              |
| Bond angles rmsd (°)           | 0.88                              | 1.68                               |
| Mean B value (Å²)              | 53                                | 52                                 |
| Number of protein atoms        | 9023                              | 9023                               |
| Mean B value for protein atoms (Å²) | 53                        | 52                                 |
| Number of water atoms (expected) | 405 (2846)                | 405 (2846)                         |
| Mean B value for water atoms (Å²) | 45                                | 47                                 |
| Number of ligand/ion atoms     | 117                               | 117                                |
| Mean B value for ligand/ion atoms (Å²) | 66                        | 70                                 |
| Clashscore                     | 4.70                              | 4.69                               |
| Clashscore percentile (100)    | -1                                | -1                                 |
| Rotamer outliers (<1%)         | 3.62                              | 3.62                               |
| Ramachandran outliers (<0.2%)  | 0.69                              | 0.69                               |
| Ramachandran favored (>98%)    | 95.52                             | 95.52                              |
| Residues with bad bonds (<0%)  | 0.05                              | 0.10                               |
| Residues with bad angles (<0.1%) | 0.10                        | 0.10                               |
| MolProbity score               | 1.98                              | 1.98                               |

---

Map cc barchart:
Small molecules with map:
Small molecule 1: GLYCEROL (GOL) A 301 map cc 0.94

Small molecule 2: GLYCEROL (GOL) A 302 map cc 0.85

Small molecule 3: GLYCEROL (GOL) A 303 map cc 0.68

Small molecule 4: GLYCEROL (GOL) A 304 map cc 0.85
Small molecule 5: GLYCEROL (GOL) A 305 map cc 0.87

Small molecule 6: GLYCEROL (GOL) A 306 map cc 0.73

Small molecule 7: GLYCEROL (GOL) A 307 map cc 0.94

Small molecule 8: GLYCEROL (GOL) B 301 map cc 0.72
Small molecule 9: GLYCEROL (GOL) B 302 map cc 0.91

Small molecule 10: GLYCEROL (GOL) B 303 map cc 0.92

Small molecule 11: GLYCEROL (GOL) G 201 map cc 0.92

Small molecule 12: GLYCEROL (GOL) G 202 map cc 0.78
Small molecule 13: GLYCEROL (GOL) H 301 map cc 0.90

Small molecule 14: GLYCEROL (GOL) H 302 map cc 0.83

Small molecule 15: GLYCEROL (GOL) H 303 map cc 0.85

Small molecule 16: GLYCEROL (GOL) L 302 map cc 0.93
Small molecule 17: GLYCEROL (GOL) L 303 map cc 0.83

Small molecule 18: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) L 301 map cc 0.93

Credits:

HKL-3000
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Model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/5t6l/structure_mr/build_model_2/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/most_twisted/5t6l/structure_mr/build_model_2/hkl_refine_34.pdb_tls

| **Data collection** | 5T6L Resolution (Å) | 47.14 - 2.10 (2.15 - 2.10) | Re-refinement Resolution (Å) | 47.14 - 2.10 |
|---------------------|---------------------|-----------------------------|-----------------------------|---------------|
| Wavelength (Å)      | 1.03314             |                             |                             |               |
| Space group         | P21                 |                             |                             |               |
| a, b, c (Å)         | 41.10, 158.97, 99.69| 41.10, 158.97, 99.69         |                             |               |
| α, β, γ (°)         | 90, 97.98, 90       | 90, 97.98, 90               |                             |               |
| Completeness (%)    | 97.5 (91.9)         |                             | 100.0 (100.0)               |               |
| Reflections used    | 72210               |                             |                             |               |
| <I> / <Sigma I>     | 9.3 (1.6)           |                             |                             |               |
| Redundancy          | 2.4 (2.3)           |                             |                             |               |
| Rmerge              | 0.074               |                             |                             |               |
| Rcryst              |                     |                             |                             |               |
| CC1/2 last shell    |                     |                             |                             |               |
| Wilson B factor (Å²)| 31.3                |                             |                             |               |

| **Refinement**      | 5T6L Rwork / Rfree | 0.178 / 0.218               | Re-refinement Rwork / Rfree | 0.199 / 0.237 |
|---------------------|------------------|----------------------------|----------------------------|---------------|
| Resolution (Å)      | 47.14 - 2.10     | 47.14 - 2.10               |                             |               |
| Reflections all     | 72183            | 72118                      |                             |               |
| Reflections for Rfree | 3620, 5.0%       | 3615, 5.0%                 |                             |               |
| Bond lengths rmsd (Å)| 0.008            | 0.013                      |                             |               |
| Bond angles rmsd (°) | 0.88             | 2.29                       |                             |               |
| Mean B value (Å²)   | 53               | 50                         |                             |               |
| Number of protein atoms | 9023            | 8878                       |                             |               |
| Mean B value for protein atoms (Å²) | 53 | 50 |
| Number of water atoms (expected) | 405 (2846) | 391 (2846) |
| Mean B value for water atoms (Å²) | 45 | 45 |
| Number of ligand/ion atoms | 117 | 117 |
| Mean B value for ligand/ion atoms (Å²) | 66 | 67 |
| Clashscore          | 4.70             | 3.13                       |                             |               |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 3.62 | 2.63 |
| Ramachandran outliers (<0.2%) | 0.69 | 0.17 |
| Ramachandran favored (>98%) | 95.52 | 97.31 |
| Residues with bad bonds (<0%) | 0.05 | 0.91 |
| Residues with bad angles (<0.1%) | 0.10 | 3.04 |
| MolProbity score    | 1.98             | 1.55                       |                             |               |

**Map cc barchart:**
Small molecules with map:
Small molecule 1: GLYCEROL (GOL) H 301 map cc 0.85

Small molecule 2: GLYCEROL (GOL) H 302 map cc 0.85

Small molecule 3: GLYCEROL (GOL) H 303 map cc 0.87

Small molecule 4: 4-(2-HYDROXYETHYL)-1-PIPRAZINEETHANESULFONICACID (EPE) L 301 map cc 0.91
Small molecule 5: GLYCEROL (GOL) L 302 map cc 0.90

Small molecule 6: GLYCEROL (GOL) L 303 map cc 0.80

Small molecule 7: GLYCEROL (GOL) A 301 map cc 0.89

Small molecule 8: GLYCEROL (GOL) A 302 map cc 0.76
Small molecule 9: GLYCEROL (GOL) A 303 map cc 0.78

Small molecule 10: GLYCEROL (GOL) A 304 map cc 0.80

Small molecule 11: GLYCEROL (GOL) A 305 map cc 0.88

Small molecule 12: GLYCEROL (GOL) A 306 map cc 0.77
Small molecule 13: GLYCEROL (GOL) A 307 map cc 0.91

Small molecule 14: GLYCEROL (GOL) B 301 map cc 0.57

Small molecule 15: GLYCEROL (GOL) B 302 map cc 0.91

Small molecule 16: GLYCEROL (GOL) B 303 map cc 0.86
Small molecule 17: GLYCEROL (GOL) G 201 map cc 0.81

Small molecule 18: GLYCEROL (GOL) G 202 map cc 0.83

Credits:

HKL-3000
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Acta Cryst. D67, 355-367 (2011)
Data collection and refinement statistics for project **hepes_6bb0** crystal **crystal1**

```markdown
| Data collection                  | 6bb0             | Re-refinement          |
|---------------------------------|------------------|------------------------|
| Resolution (Å)                  | 39.00 - 1.95 (2.05 - 1.95) | 47.01 - 1.95          |
| Wavelength (Å)                  | 0.9795           |                        |
| Space group                     | P21              | P21                    |
| a, b, c (Å)                     | 78.12, 80.97, 103.21 | 78.12, 80.97, 103.21   |
| α, β, γ (°)                     | 90, 98.33, 90    | 90, 98.33, 90          |
| Completeness (%)                | 97.8 (95.9)      | 97.9 (97.3)            |
| Reflections used                | 91115            |                        |
| <I> / <Sigma I>                 | 16.6 (2.3)       |                        |
| Redundancy                      | 3.4 (3.4)        |                        |
| Rmerge                          | 0.046 (0.491)    |                        |
| Wilson B factor (Å²)            |                  | 32.1                   |

**Refinement**

| Rwork / Rfree                   | 0.166 / 0.215 | 0.172 / 0.211 |
| Resolution (Å)                  | 38.65 - 1.95  | 38.68 - 1.95   |
| Reflections all                 | 89114          | 90971          |
| Reflections for Rfree           | 1830, 2.0%     | 1830, 2.0%     |
| Bond lengths rmsd (Å)           | 0.010          | 0.017          |
| Bond angles rmsd (°)            | 1.51           | 1.94           |
| Mean B value (Å²)               | 38             | 36             |
| Number of protein atoms         | 10132          | 10132          |
| Mean B value for protein atoms (Å²) | 37          | 36             |
| Number of water atoms (expected)| 721 (1187)     | 721 (1187)     |
| Mean B value for water atoms (Å²)| 37          | 38             |
| Number of ligand/ion atoms      | 334            | 334            |
| Mean B value for ligand/ion atoms (Å²)| 45          | 44             |
| Clashscore                      | 1.89           | 1.89           |
| Clashscore percentile (100)     | -1             | -1             |
| Rotamer outliers (<1%)          | 0.97           | 0.97           |
| Ramachandran outliers (<0.2%)   | 0.16           | 0.16           |
| Ramachandran favored (>98%)     | 98.05          | 98.05          |
| Residues with bad bonds (<0%)   | 0.12           | 0.12           |
| Residues with bad angles (<0.1%)| 0.35           | 0.15           |
| MolProbity score                | 0.95           | 0.95           |

Map cc barchart:
Small molecules with map:
Small molecule 1: NICOTINAMIDE-ADENINE-DINUCLEOTIDE (NAD) A 801 map cc 0.96

Small molecule 2: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 802 map cc 0.88

Small molecule 3: SULFATE ION (SO4) A 803 map cc 0.98

Small molecule 4: (6S)-3-[(2-chlorophenyl)sulfanyl]-4-hydroxy-6-(2-hydroxyphenyl)-6-phenyl-5,6-dihydro-2H-pyran-2-one (D3S) A 804 map cc 0.92
Small molecule 5: NICOTINAMIDE-ADENINE-DINUCLEOTIDE (NAD) B 801 map cc 0.98

Small molecule 6: 4-(2-HYDROXYETHYL)-1-PIPRAZINEETHANESULFONICACID (EPE) B 802 map cc 0.93

Small molecule 7: SULFATE ION (SO4) B 803 map cc 0.94

Small molecule 8: LACTIC ACID (LAC) B 804 map cc 0.95
Small molecule 9: NICOTINAMIDE-ADENINE-DINUCLEOTIDE (NAD) C 801 map cc 0.96

Small molecule 10: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) C 802 map cc 0.78

Small molecule 11: SULFATE ION (SO4) C 803 map cc 0.97

Small molecule 12: (6S)-3-[(2-chlorophenyl)sulfanyl]-4-hydroxy-6-(2-hydroxyphenyl)-6-phenyl-5,6-dihydro-2H-pyran-2-one (D3S) C 804 map cc 0.90
Small molecule 13: NICOTINAMIDE-ADENINE-DINUCLEOTIDE (NAD) D 801 map cc 0.98

Small molecule 14: (6S)-3-[(2-chlorophenyl)sulfanyl]-4-hydroxy-6-(2-hydroxyphenyl)-6-phenyl-5,6-dihydro-2H-pyran-2-one (D3S) D 802 map cc 0.96

Small molecule 15: SULFATE ION (SO4) D 803 map cc 0.97

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HKL-3000
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P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **hepes_6bb0** crystal **crystal1**

| Data collection | 6BB0 | Re-refinement |
|-----------------|------|--------------|
| Resolution (Å)  | 39.00 - 1.95 (2.05 - 1.95) | 47.01 - 1.95 |
| Wavelength (Å)  | 0.9795 |               |
| Space group     | P21  | P21          |
| a, b, c (Å)     | 78.12, 80.97, 103.21 | 78.12, 80.97, 103.21 |
| α, β, γ (°)     | 90, 98.33, 90 | 90, 98.33, 90 |
| Completeness (%)| 97.8 (95.9) | 97.9 (97.3) |
| Reflections used| 91115 |              |
| <I> / <Sigma I> | 16.6 (2.3) |              |
| Redundancy      | 3.4 (3.4) |              |
| Rmerge          | 0.046 (0.491) |           |
| Wilson B factor (Å²) | 32.1 |           |

| Refinement |
|------------|
| Rwork / Rfree | 0.166 / 0.215 | 0.162 / 0.205 |
| Resolution (Å) | 38.65 - 1.95 | 38.68 - 1.95 |
| Refractions all | 89141 | 90971 |
| Reflections for Rfree | 1830, 2.0% | 1830, 2.0% |
| Bond lengths rmsd (Å) | 0.010 | 0.013 |
| Bond angles rmsd (°) | 1.51 | 1.80 |
| Mean B value (Å²) | 38 | 37 |
| Number of protein atoms | 10132 | 10113 |
| Mean B value for protein atoms (Å²) | 37 | 37 |
| Number of water atoms (expected) | 721 (1187) | 724 (1187) |
| Mean B value for water atoms (Å²) | 37 | 39 |
| Number of ligand/ion atoms | 334 | 334 |
| Mean B value for ligand/ion atoms (Å²) | 45 | 44 |
| Clashscore | 1.89 | 2.70 |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 0.97 | 1.41 |
| Ramachandran outliers (<0.2%) | 0.16 | 0.08 |
| Ramachandran favored (>98%) | 98.05 | 97.66 |
| Residues with bad bonds (<5%) | 0.12 | 0.38 |
| Residues with bad angles (<0.1%) | 0.35 | 1.31 |
| MolProbity score | 0.95 | 1.24 |

**Map cc barchart:**
Small molecules with map:
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Small molecule 2: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 802 map cc 0.90

Small molecule 3: SULFATE ION (SO4) A 803 map cc 0.98

Small molecule 4: (6S)-3-[(2-chlorophenyl)sulfanyl]-4-hydroxy-6-(2-hydroxyphenyl)-6-phenyl-5,6-dihydro-2H-pyran-2-one (D3S) A 804 map cc 0.90
Small molecule 5: NICOTINAMIDE-ADENINE-DINUCLEOTIDE (NAD) B 801 map cc 0.98

Small molecule 6: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) B 802 map cc 0.93

Small molecule 7: SULFATE ION (SO4) B 803 map cc 0.96

Small molecule 8: LACTIC ACID (LAC) B 804 map cc 0.97
Small molecule 9: NICOTINAMIDE-ADENINE-DINUCLEOTIDE (NAD) C 801 map cc 0.96

Small molecule 10: 4-(2-HYDROXYETHYL)-1-PIPRAZINEETHANESULFONICACID (EPE) C 802 map cc 0.87

Small molecule 11: SULFATE ION (SO4) C 803 map cc 0.97

Small molecule 12: (6S)-3-[(2-chlorophenyl)sulfanyl]-4-hydroxy-6-(2-hydroxyphenyl)-6-phenyl-5,6-dihydro-2H-pyran-2-one (D3S) C 804 map cc 0.92
Small molecule 13: NICOTINAMIDE-ADENINE-DINUCLEOTIDE (NAD) D 801 map cc 0.98

Small molecule 14: (6S)-3-{(2-chlorophenyl)sulfanyl}-4-hydroxy-6-(2-hydroxyphenyl)-6-phenyl-5,6-dihydro-2H-pyran-2-one (D3S) D 802 map cc 0.96

Small molecule 15: SULFATE ION (SO4) D 803 map cc 0.97

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P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
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Data collection and refinement statistics for project **mes_3o4p crystal crystal1**

model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3o4p/structure_mr/build_model_2/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3o4p/structure_mr/build_model_2/hkl_refine_496.pdb

### Data collection

| Resolution (Å)   | 3O4P  | Re-refinement |
|------------------|-------|---------------|
| Resolution (Å)   | 20.80 - 0.85 (-) | 20.92 - 0.83 |
| Wavelength (Å)   | 0.842 |               |
| Space group      | P212121 | P212121       |
| a, b, c (Å)      | 43.11, 81.85, 86.47 | 43.11, 81.85, 86.47 |
| α, β, γ (°)      | 90, 90, 90 | 90, 90, 90   |
| Completeness (%) | 93.8  | 100.0 (100.0) |
| Reflections used | 264548 |               |
| ⦰ / <Sigma I>    |       |               |
| Redundancy       |       |               |
| Rmerge           |       |               |
| Rpim             |       |               |
| Wilson B factor (Å²) | 5.9  |               |

### Refinement

| Rwork / Rfree | 0.103 / 0.121 | 0.123 / 0.136 |
| Resolution (Å) | 20.80 - 0.85 | 20.92 - 0.83 |
| Reflections all | 241251  | 255775       |
| Reflections for Rfree | 2463, % | 2584, 1.0% |
| Bond lengths rmsd (Å) |       | 0.037        |
| Bond angles rmsd (°)  |       | 3.60         |
| Mean B value (Å²)    | 12     | 12           |
| Number of protein atoms | 2657    | 2657         |
| Mean B value for protein atoms (Å²) | 10 | 9 |
| Number of water atoms (expected) | 481 (572) | 481 (572) |
| Mean B value for water atoms (Å²) | 21 | 21 |
| Number of ligand/ion atoms | 136 | 136 |
| Mean B value for ligand/ion atoms (Å²) | 29 | 30 |
| Clashscore | 29.10 | 28.22 |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 1.30 | 1.30 |
| Ramachandran outliers (<0.2%) | 0.32 | 0.32 |
| Ramachandran favored (>98%) | 96.15 | 96.15 |
| Residues with bad bonds (<0%) | 5.69 | 5.53 |
| Residues with bad angles (<0.1%) | 9.13 | 8.97 |
| MolProbity score | 2.30 | 2.29 |

### Map cc barchart:
Small molecules with map:

Small molecule 1: GLYCEROL (GOL) A 401 map cc 0.95

Small molecule 2: GLYCEROL (GOL) A 403 map cc 0.91
Small molecule 3: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 411 map cc 0.80

Small molecule 4: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 412 map cc 0.82

Small molecule 5: 1,2-ETHANEDIOL (EDO) A 421 map cc 0.93

Small molecule 6: 1,2-ETHANEDIOL (EDO) A 422 map cc 0.95
Small molecule 11: 1,2-ETHANEDIOL (EDO) A 427 map cc 0.88

Small molecule 12: 1,2-ETHANEDIOL (EDO) A 428 map cc 0.90

Small molecule 13: TRIETHYLENE GLYCOL (PGE) A 433 map cc 0.88

Small molecule 14: TRIETHYLENE GLYCOL (PGE) A 434 map cc 0.92
Small molecule 15: 1,2-DIMETHOXYETHANE (DXE) A 442 map cc 0.77

Small molecule 16: 1,2-DIMETHOXYETHANE (DXE) A 443 map cc 0.77

Small molecule 17: 2-METHOXYETHANOL (MXE) A 451 map cc 0.93

Small molecule 18: 2-METHOXYETHANOL (MXE) A 452 map cc 0.95
Small molecule 19: DI(HYDROXYETHYL)ETHER (PEG) A 461 map cc 0.56

Small molecule 20: 1-ETHOXY-2-(2-METHOXYETHOXY)ETHANE (ME2) A 471 map cc 0.75

Small molecule 21: CALCIUM ION (CA) A 491 map cc 1.00

Small molecule 22: CALCIUM ION (CA) A 492 map cc 1.00
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**model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3o4p/structure_mr/build_model_2/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3o4p/structure_mr/build_model_2/hkl_refine_501.pdb**

| Data collection | 3O4P | Re-refinement |
|-----------------|------|---------------|
| Resolution (Å)  | 20.80 - 0.85 (-) | 20.92 - 0.83 |
| Wavelength (Å)  | 0.842 | |
| Space group     | P212121 | P212121 |
| a, b, c (Å)     | 43.11, 81.85, 86.47 | 43.11, 81.85, 86.47 |
| α, β, γ (°)     | 90, 90, 90 | 90, 90, 90 |
| ComPLEteness (%)| 93.8 | 100.0 (100.0) |
| Reflections used| 264548 | |
| <I> / <Sigma I> | |
| Redundancy      | |
| Rmerge          | |
| Rpim            | |
| CC1/2 last shell| |
| Wilson B factor (Å²) | 5.9 | |

**ReFINEMENT**

| Rwork / Rfree   | 0.103 / 0.121 | 0.120 / 0.131 |
| Resolution (Å)  | 20.80 - 0.85 | 20.92 - 0.83 |
| Reflections all | 241251 | 255775 |
| Reflections for Rfree | 2463, % | 2584, 1.0% |
| Bond lengths rmsd (Å) | | 0.035 |
| Bond angles rmsd (°) | | 2.50 |
| Mean B value (Å²) | 12 | 11 |
| Number of protein atoms | 2657 | 2638 |
| Mean B value for protein atoms (Å²) | 10 | 8 |
| Number of water atoms (expected) | 481 (572) | 484 (572) |
| Mean B value for water atoms (Å²) | 21 | 19 |
| Number of ligand/ion atoms | 136 | 129 |
| Mean B value for ligand/ion atoms (Å²) | 29 | 24 |
| Clashscore | 29.10 | 18.70 |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 1.30 | 1.63 |
| Ramachandran outliers (<0.2%) | 0.32 | 0.00 |
| Ramachandran favored (>98%) | 96.15 | 96.14 |
| Residues with bad bonds (<0%) | 5.69 | 1.07 |
| Residues with bad angles (<0.1%) | 9.13 | 4.70 |
| MolProbity score | 2.30 | 2.19 |

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Small molecule 7: 1,2-ETHANEDIOL (EDO) A 423 map cc 0.81

Small molecule 8: 1,2-ETHANEDIOL (EDO) A 424 map cc 0.95

Small molecule 9: 1,2-ETHANEDIOL (EDO) A 425 map cc 0.93

Small molecule 10: 1,2-ETHANEDIOL (EDO) A 426 map cc 0.93
Small molecule 11: 1,2-ETHANEDIOL (EDO) A 427 map cc 0.88

Small molecule 12: 1,2-ETHANEDIOL (EDO) A 428 map cc 0.90

Small molecule 13: TRIETHYLENE GLYCOL (PGE) A 433 map cc 0.88

Small molecule 14: TRIETHYLENE GLYCOL (PGE) A 434 map cc 0.92
Small molecule 15: 1,2-DIMETHOXYETHANE (DXE) A 442 map cc 0.77

Small molecule 16: 1,2-DIMETHOXYETHANE (DXE) A 443 map cc 0.77

Small molecule 17: 2-METHOXYETHANOL (MXE) A 451 map cc 0.93

Small molecule 18: 2-METHOXYETHANOL (MXE) A 452 map cc 0.95
Small molecule 19: DI(HYDROXYETHYL)ETHER (PEG) A 461 map cc 0.56

Small molecule 20: 1-ETHOXY-2-(2-METHOXYETHOXY)ETHANE (ME2) A 471 map cc 0.75

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Coot
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Acta Cryst. D66, 486-501 (2010)
**Data collection**

|                          | 6WCF          | Re-refinement |
|--------------------------|---------------|---------------|
| Resolution (Å)           | 50.00 - 1.06  | 60.27 - 0.73  |
| Wavelength (Å)           | 0.97918       | P21           |
| Space group              | P21           | P21           |
| a, b, c (Å)              | 37.17, 33.18, 60.62 | 37.17, 33.18, 60.62 |
| α, β, γ (*)              | 90, 96.11, 90 | 90, 96.11, 90 |
| Completeness (%)         | 97.9 (94.8)   | 83.8 (0.0)    |
| Reflections used         | 64283         |               |
| <I> / <Sigma I>          | 18.7 (1.5)    |               |
| Redundancy               | 5.9 (3.9)     |               |
| Rmerge                    | 0.094         |               |
| Wilson B factor (Å²)     |               | 8.9           |

**Refinement**

|                          | 0.125 / 0.154 | 0.135 / 0.161 |
|--------------------------|---------------|---------------|
| Resolution (Å)           | 33.13 - 1.06  | 33.14 - 1.06  |
| Reflections all          | 64228         | 64261         |
| Reflections for Rfree    | 3250, 5.1%    | 3252, 5.1%    |
| Bond lengths rmsd (Å)    | 0.012         | 0.018         |
| Bond angles rmsd (*)     | 1.41          | 1.98          |
| Mean B value (Å²)        | 16            | 16            |
| Number of protein atoms  | 1413          | 1413          |
| Mean B value for protein atoms (Å²) | 14 | 14 |
| Number of water atoms (expected) | 197 (323) | 197 (323) |
| Mean B value for water atoms (Å²) | 31 | 30 |
| Number of ligand/ion atoms | 24      | 24            |
| Mean B value for ligand/ion atoms (Å²) | 23 | 25 |
| Clashscore               | 4.12          | 4.12          |
| Clashscore percentile (100) | -1        | -1            |
| Rotamer outliers (<1%)   | 0.64          | 0.64          |
| Ramachandran outliers (<0.2%) | 0.00      | 0.00          |
| Ramachandran favored (>98%) | 100.00     | 100.00        |
| Residues with bad bonds (<0%) | 0.00       | 0.30          |
| Residues with bad angles (<0.1%) | 0.00      | 0.30          |
| MolProbity score         | 1.20          | 1.20          |

**Map cc barchart:**

**Small molecules with map:**
Small molecule 1: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 201 map cc 0.99

Small molecule 2: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 202 map cc 0.93

Credits:

HKL-3000
"Processing of X-ray Diffraction Data Collected in Oscillation Mode"
Z.Otwinowski, W.Minor
Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p307-326 (1997)

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Acta Cryst. D62: 859-866 (2006)

CCP4 suite
"Overview of the CCP4 suite and current developments"
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Acta. Cryst. D67, 235-242 (2011)

Refmac5
"REFMAC5 for the refinement of macromolecular crystal structures"
G.N.Murshudov, P.Skubak, A.A.Lebedev, N.S.Pannu, R.A.Steiner, R.A.Nicholls, M.D.Winn, F.Long and A.A.Vagin
Acta Cryst. D67, 355-367 (2011)
Data collection and refinement statistics for project **mes_6wcf crystal crystal1**

model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/6wcf/structure_mr/build_model_1/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/6wcf/structure_mr/build_model_1/hkl_refine_203.pdb

| Data collection                                                                 | 6WCF                  | Re-refinement                  |
|--------------------------------------------------------------------------------|-----------------------|--------------------------------|
| Resolution (Å)                                                                 | 50.00 - 1.06 (1.09 - 1.06) | 60.27 - 0.73                  |
| Wavelength (Å)                                                                | 0.97918               |                                |
| Space group                                                                    | P21                   | P21                            |
| a, b, c (Å)                                                                   | 37.17, 33.18, 60.62   | 37.17, 33.18, 60.62            |
| α, β, γ (*)                                                                    | 90, 96.11, 90         | 90, 96.11, 90                  |
| Completeness (%)                                                               | 97.9 (94.8)           | 83.8 (0.0)                     |
| Reflections used                                                              | 64283                 |                                |
| <I> / <Sigma I>                                                               | 18.7 (1.5)            |                                |
| Redundancy                                                                     | 5.9 (3.9)             |                                |
| Rmerge                                                                        | 0.094                 |                                |
| Wilson B factor (Å²)                                                           | 8.9                   |                                |

**Refinement**

| Rwork / Rfree                                                                 | 0.125 / 0.154         | 0.134 / 0.160                  |
| Resolution (Å)                                                                | 33.13 - 1.06          | 33.14 - 1.06                   |
| Reflections all                                                               | 64228                 | 64261                          |
| Reflections for Rfree                                                         | 3250, 5.1%            | 3252, 5.1%                     |
| Bond lengths rmsd (Å)                                                         | 0.012                 | 0.019                          |
| Bond angles rmsd (*)                                                          | 1.41                  | 2.06                           |
| Mean B value (Å²)                                                             | 16                    | 17                             |
| Number of protein atoms                                                       | 1413                  | 1413                           |
| Mean B value for protein atoms (Å²)                                           | 14                    | 15                             |
| Number of water atoms (expected)                                             | 197 (323)             | 197 (323)                      |
| Mean B value for water atoms (Å²)                                             | 31                    | 30                             |
| Number of ligand/ion atoms                                                   | 24                    | 24                             |
| Mean B value for ligand/ion atoms (Å²)                                        | 23                    | 25                             |
| Clashscore                                                                    | 4.12                  | 4.46                           |
| Clashscore percentile (100)                                                   | -1                   | -1                             |
| Rotamer outliers (<1%)                                                        | 0.64                  | 0.64                           |
| Ramachandran outliers (<0.2%)                                                | 0.00                  | 0.00                           |
| Ramachandran favored (>98%)                                                  | 100.00                | 100.00                         |
| Residues with bad bonds (<0%)                                                | 0.00                  | 0.90                           |
| Residues with bad angles (<0.1%)                                             | 0.00                  | 1.81                           |
| MolProbity score                                                             | 1.20                  | 1.22                           |

**Map cc barchart:**

Chain A

NDFGSVLKLTQNVYFKNADIVKEAKRVRFTVTVVNAANNYVLRHGGVA
GALNKATNMAMGVESSDYIATNGPLKVG5CVLSLSRMHNLKACHLHVVG
PNVKGEDIQLLLKASAYENFQNSHEVLLAPLLSSAAGIFGADFIPHSILRVCV
DVTNIVYLAFTDNLLODYKLVGGSF

Chain A - small molecules: MES

- Water molecules

Legend

| Value | Color |
|-------|-------|
| > 0.95 | Green |
| > 0.9  | Orange|
| > 0.8  | Yellow|
| > 0.7  | Red   |
| > 0.6  | Brown |
| <= 0.6 | Gray  |

**Small molecules with map:**
Small molecule 1: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 201 map cc 0.99

Small molecule 2: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 202 map cc 0.93

Credits:

HKL-3000
"Processing of X-ray Diffraction Data Collected in Oscillation Mode"
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Refmac5
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Acta Cryst. D67, 355-367 (2011)
Coot
"Features and Development of Coot"
P. Emsley, B. Lohkamp, W. Scott, and K. Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **hepes_3dke** crystal **crystal1**

| Data collection | 3DKE | Re-refinement |
|-----------------|------|---------------|
| Resolution (Å)  | 52.20 - 1.25 (1.27 - 1.25) | 52.16 - 1.25 |
| Wavelength (Å)  | 0.9796, 0.9797, 0.9742, 0.9807 | |
| Space group     | P3221 | P3221 |
| a, b, c (Å)     | 60.23, 60.23, 96.68 | 60.23, 60.23, 96.68 |
| α, β, γ (°)     | 90, 90, 120 | 90, 90, 120 |
| Completeness (%)| 99.9 (100.0) | 100.0 (100.0) |
| Reflections used| 56299 | |
| <I>/<Sigma I>   | 23.2 (13.9) | |
| Redundancy      | 9.6 (7.1) | |
| Rmerge          | 0.115 | |
| Rfree           | |
| Wilson B factor (Å²) | 10.9 | |

**Refinement**

|                | 0.155 / 0.173 | 0.169 / 0.173 |
|----------------|---------------|---------------|
| Rwork / Rfree | 52.13 - 1.25  | 52.16 - 1.25  |
| Reflections all| 53423 | 56108 |
| Reflections for Rfree| 2851, 5.1% | 2789, 5.0% |
| Bond lengths rmsd (Å) | 0.007 | 0.016 |
| Bond angles rmsd (°) | 1.14 | 1.89 |
| Mean B value (Å²) | 15 | 14 |
| Number of protein atoms | 1334 | 1334 |
| Mean B value for protein atoms (Å²) | 12 | 12 |
| Number of water atoms (expected) | 256 (242) | 256 (242) |
| Mean B value for water atoms (Å²) | 27 | 24 |
| Number of ligand/ion atoms | 57 | 57 |
| Mean B value for ligand/ion atoms (Å²) | 22 | 25 |
| Clashscore | 4.24 | 4.24 |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 0.00 | 0.00 |
| Ramachandran outliers (<0.2%) | 0.00 | 0.00 |
| Ramachandran favored (>98%) | 97.53 | 97.53 |
| Residues with bad bonds (<0%) | 0.00 | 0.30 |
| Residues with bad angles (<0.1%) | 0.30 | 0.61 |
| MolProbity score | 1.30 | 1.30 |

**Map cc barchart:**

```
Chain X

Legend
> 0.95  > 0.9  > 0.8  > 0.7  > 0.6  <= 0.6

Small molecules with map:
```
Small molecule 1: POTASSIUM ION (K) X 601 map cc 0.99

Small molecule 2: CHLORIDE ION (CL) X 701 map cc 0.99

Small molecule 3: CHLORIDE ION (CL) X 702 map cc 0.99

Small molecule 4: AZIDE ION (AZI) X 401 map cc 0.98
Small molecule 5: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) X 901 map cc 0.86

Small molecule 6: BETA-MERCAPTOETHANOL (BME) X 805 map cc 0.86

Small molecule 7: BETA-MERCAPTOETHANOL (BME) X 806 map cc 0.89

Small molecule 8: 2-HYDROXYETHYL DISULFIDE (HED) X 801 map cc 0.93
Small molecule 9: 2-HYDROXYETHYL DISULFIDE (HED) X 802 map cc 0.91

Small molecule 10: GLYCEROL (GOL) X 501 map cc 0.82

Small molecule 11: GLYCEROL (GOL) X 502 map cc 0.70

Credits:
HKL-3000
"Processing of X-ray Diffraction Data Collected in Oscillation Mode"
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Coot
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P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **hepes_3dke** crystal **crystal1**

Model: /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3dke/structure_mr/build_model_1/hkl_import.pdb tls vs
model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3dke/structure_mr/build_model_1/hkl_refine_13.pdb

### Data collection

|                      | 3DKE                  | Re-refinement          |
|----------------------|-----------------------|------------------------|
| Resolution (Å)       | 52.20 - 1.25 (1.27 - 1.25) | 52.16 - 1.25            |
| Wavelength (Å)       | 0.9796, 0.9797, 0.9742, 0.9807 |                       |
| Space group          | P3221                 | P3221                  |
| a, b, c (Å)          | 60.23, 60.23, 96.68   | 60.23, 60.23, 96.68    |
| α, β, γ (*)          | 90, 90, 120           | 90, 90, 120            |
| Completeness (%)     | 99.9 (100.0)          | 100.0 (100.0)          |
| Reflections used     | 56299                 |                        |
| <I> / <Sigma I>     | 23.2 (13.9)           |                        |
| Redundancy           | 9.6 (7.1)             |                        |
| Rmerge               | 0.115                 |                        |
| Rpim                 |                       |                        |
| Wilson B factor (Å²) | 10.9                  |                        |

### Refinement

|                      | 3DKE                  | Re-refinement          |
|----------------------|-----------------------|------------------------|
| Rwork / Rfree        | 0.155 / 0.173         | 0.160 / 0.175          |
| Resolution (Å)       | 52.13 - 1.25          | 52.16 - 1.25           |
| Reflections all      | 53423                 | 56108                  |
| Reflections for Rfree| 2851, 5.1%            | 2789, 5.0%             |
| Bond lengths rmsd (Å)| 0.007                 | 0.020                  |
| Bond angles rmsd (*) | 1.14                  | 2.40                   |
| Mean B value (Å³)    | 15                    | 14                     |
| Number of protein atoms| 1334                 | 1334                   |
| Mean B value for protein atoms (Å³)| 12         | 11                     |
| Number of water atoms (expected)| 256 (242)    | 256 (242)             |
| Mean B value for water atoms (Å³)| 27          | 24                     |
| Number of ligand/ion atoms| 57           | 57                     |
| Mean B value for ligand/ion atoms (Å³)| 22         | 24                     |
| Clashscore           | 4.24                  | 5.30                   |
| Clashscore percentile (100)| -1          | -1                     |
| Rotamer outliers (<1%)| 0.00                | 0.00                   |
| Ramachandran outliers (<0.2%)| 0.00     | 0.00                   |
| Ramachandran favored (>98%)| 97.53        | 98.15                  |
| Residues with bad bonds (<0%)| 0.00      | 1.52                   |
| Residues with bad angles (<0.1%)| 0.30       | 3.66                   |
| MolProbity score     | 1.30                  | 1.28                   |

**Map cc barchart:**

*Small molecules with map:*

![Map cc barchart](image)
Small molecule 1: POTASSIUM ION (K) X 601 map cc 0.99

Small molecule 2: CHLORIDE ION (CL) X 701 map cc 0.99

Small molecule 3: CHLORIDE ION (CL) X 702 map cc 0.99

Small molecule 4: AZIDE ION (AZI) X 401 map cc 0.98
Small molecule 5: 4-(2-HYDROXYETHYL)-1-PIPerezinesulfonylacid (EPE) X 901 map cc 0.86

Small molecule 6: BETA-MERCAPTOETHANOL (BME) X 805 map cc 0.86

Small molecule 7: BETA-MERCAPTOETHANOL (BME) X 806 map cc 0.89

Small molecule 8: 2-HYDROXYETHYL DISULFIDE (HED) X 801 map cc 0.93
Small molecule 9: 2-HYDROXYETHYL DISULFIDE (HED) X 802 map cc 0.91

Small molecule 10: GLYCEROL (GOL) X 501 map cc 0.82

Small molecule 11: GLYCEROL (GOL) X 502 map cc 0.70

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HKL-3000
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Coot
"Features and Development of Coot"
P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
**Data collection and refinement statistics for project** **hepes_3e10** **crystal crystal1**

```
model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3e10/structure_mr/build_model_1/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/3e10/structure_mr/build_model_1/hkl_refine_3.pdb
```

| Data collection | 3E10 | Re-refinement |
|-----------------|------|---------------|
| Resolution (Å)  | 29.27 - 1.40 (1.44 - 1.40) | 29.27 - 1.40 |
| Wavelength (Å)  | 0.91837, 0.97908, 0.97849 |  |
| Space group     | P21212 | P21212 |
| a, b, c (Å)     | 82.08, 83.53, 51.89 | 82.08, 83.53, 51.89 |
| α, β, γ (°)     | 90, 90, 90 | 90, 90, 90 |
| Completeness (%)| 100.0 | 100.0 (100.0) |
| Reflections used| 70997 |  |
| <I> / <Sigma I> | (1.5) |  |
| Redundancy      | 3.7 (3.6) |  |
| Rmerge          | 0.096 |  |
| Wilson B factor (Å²) | 10.6 |  |

| Refinement       | 3E10 | Re-refinement |
|------------------|------|---------------|
| Rwork / Rfree    | 0.130 / 0.168 | 0.153 / 0.157 |
| Resolution (Å)   | 29.27 - 1.40 | 29.27 - 1.40 |
| Reflections all  | 70948 | 70948 |
| Reflections for Rfree | 3583, 5.1% | 3485, 4.9% |
| Bond lengths rmsd (Å) | 0.015 | 0.019 |
| Bond angles rmsd (°) | 1.57 | 2.07 |
| Mean B value (Å²) | 13 | 14 |
| Number of protein atoms | 2860 | 2860 |
| Mean B value for protein atoms (Å²) | 11 | 11 |
| Number of water atoms (expected) | 519 (454) | 519 (454) |
| Mean B value for water atoms (Å²) | 27 | 28 |
| Number of ligand/ion atoms | 134 | 134 |
| Mean B value for ligand/ion atoms (Å²) | 16 | 17 |
| Clashscore       | 3.75 | 3.91 |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 0.96 | 0.96 |
| Ramachandran outliers (<0.2%) | 0.00 | 0.00 |
| Ramachandran favored (>98%) | 97.26 | 97.26 |
| Residues with bad bonds (<0%) | 0.30 | 0.30 |
| Residues with bad angles (<0.1%) | 0.00 | 0.00 |
| MolProbity score | 1.30 | 1.32 |

**Map cc barchart:**
Small molecules with map:

Small molecule 1: FLAVINMONONUCLEOTIDE (FMN) A 501 map cc 0.99

Small molecule 2: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 502 map cc 0.98
Small molecule 3: 1,2-ETHANEDIOL (EDO) A 503 map cc 0.96

Small molecule 4: 1,2-ETHANEDIOL (EDO) A 504 map cc 0.95

Small molecule 5: 1,2-ETHANEDIOL (EDO) A 505 map cc 0.98

Small molecule 6: 1,2-ETHANEDIOL (EDO) A 506 map cc 0.96
Small molecule 7: 1,2-ETHANEDIOL (EDO) A 507 map cc 0.94

Small molecule 8: 1,2-ETHANEDIOL (EDO) A 508 map cc 0.83

Small molecule 9: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) B 502 map cc 0.97

Small molecule 10: FLAVINMONONUCLEOTIDE (FMN) B 501 map cc 0.99
Small molecule 11: 1,2-ETHANEDIOL (EDO) B 503 map cc 0.89

Small molecule 12: 1,2-ETHANEDIOL (EDO) B 504 map cc 0.94

Small molecule 13: 1,2-ETHANEDIOL (EDO) B 505 map cc 0.87

Small molecule 14: 1,2-ETHANEDIOL (EDO) B 506 map cc 0.87
Credits:

HKL-3000
"Processing of X-ray Diffraction Data Collected in Oscillation Mode"
Z.Otwinowski, W.Minor
Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p307-326 (1997)
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Coot
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P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
### Data collection

|                      | 3E10                        | Re-refinement               |
|----------------------|-----------------------------|-----------------------------|
| Resolution (Å)       | 29.27 - 1.40 (1.44 - 1.40)  | 29.27 - 1.40                |
| Wavelength (Å)       | 0.91837, 0.97908, 0.97849   |                            |
| Space group          | P21212                      | P21212                      |
| a, b, c (Å)          | 82.08, 83.53, 51.89         | 82.08, 83.53, 51.89         |
| α, β, γ (°)          | 90, 90, 90                  | 90, 90, 90                  |
| Completeness (%)     | 100.0                       | 100.0 (100.0)               |
| Reflections used     |                            | 70997                       |
| <I> / <Sigma I>      | (1.5)                       |                            |
| Redundancy           | 3.7 (3.6)                   |                            |
| Rmerge               | 0.096                       |                            |
| Rpim                 |                            |                            |
| CC1/2 last shell     |                            |                            |
| Wilson B factor (Å²) |                            | 10.6                        |

### Refinement

|                      | 3E10                        | Re-refinement               |
|----------------------|-----------------------------|-----------------------------|
| Rwork / Rfree        | 0.130 / 0.168               | 0.149 / 0.166               |
| Resolution (Å)       | 29.27 - 1.40                | 29.27 - 1.40                |
| Reflections all      | 70948                       | 70948                       |
| Reflections for Rfree| 3583, 5.1%                  | 3485, 4.9%                  |
| Bond lengths rmsd (Å)| 0.015                       | 0.015                       |
| Bond angles rmsd (°)  | 1.57                        | 1.96                        |
| Mean B value (Å²)    | 13                          | 14                          |
| Number of protein atoms | 2860                      | 2860                       |
| Mean B value for protein atoms (Å²) | 11                        | 11                        |
| Number of water atoms (expected) | 519 (454) | 519 (454) |
| Mean B value for water atoms (Å²) | 27                        | 28                          |
| Number of ligand/ion atoms | 134                       | 134                         |
| Mean B value for ligand/ion atoms (Å²) | 16                        | 17                          |
| Clashscore           | 3.75                        | 3.42                        |
| Clashscore percentile (100) | -1                       | -1                          |
| Rotamer outliers (<1%)  | 0.96                        | 0.64                        |
| Ramachandran outliers (<0.2%)  | 0.00                        | 0.00                        |
| Ramachandran favored (>98%) | 97.26                      | 97.26                       |
| Residues with bad bonds (<0%) | 0.30                      | 0.75                        |
| Residues with bad angles (<0.1%) | 0.00                      | 1.05                        |
| MolProbity score     | 1.30                        | 1.27                        |

### Map cc barchart:
Small molecules with map:

Small molecule 1: FLAVINMONONUCLEOTIDE (FMN) A 501 map cc 0.99

Small molecule 2: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 502 map cc 0.98
Small molecule 3: 1,2-ETHANEDIOL (EDO) A 503 map cc 0.97

Small molecule 4: 1,2-ETHANEDIOL (EDO) A 504 map cc 0.95

Small molecule 5: 1,2-ETHANEDIOL (EDO) A 505 map cc 0.98

Small molecule 6: 1,2-ETHANEDIOL (EDO) A 506 map cc 0.96
Small molecule 7: 1,2-ETHANEDIOL (EDO) A 507 map cc 0.97

Small molecule 8: 1,2-ETHANEDIOL (EDO) A 508 map cc 0.89

Small molecule 9: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) B 502 map cc 0.97

Small molecule 10: FLAVINMONONUCLEOTIDE (FMN) B 501 map cc 0.99
Small molecule 11: 1,2-ETHANEDIOL (EDO) B 503 map cc 0.91

Small molecule 12: 1,2-ETHANEDIOL (EDO) B 504 map cc 0.96

Small molecule 13: 1,2-ETHANEDIOL (EDO) B 505 map cc 0.89

Small molecule 14: 1,2-ETHANEDIOL (EDO) B 506 map cc 0.81
Credits:

HKL-3000
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Coot
"Features and Development of Coot"
P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
### Data collection and refinement statistics for project `hepes_6g38` crystal `crystal1`

|                      | 6G38               | Re-refinement          |
|----------------------|--------------------|------------------------|
| Resolution (Å)       | 24.05 - 1.43 (1.45 - 1.43) | 56.13 - 1.47           |
| Wavelength (Å)       | 0.9794             |                        |
| Space group          | P212121            | P212121                |
| a, b, c (Å)          | 78.56, 78.76, 80.02 | 78.56, 78.76, 80.02    |
| α, β, γ (°)          | 90, 90, 90         | 90, 90, 90             |
| Completeness (%)     | 99.9 (98.3)        | 100.0 (100.0)          |
| Reflections used     | 92144              |                        |
| <I> / <Sigma I>      | 8.6 (1.2)          |                        |
| Redundancy           | 5.9 (4.2)          |                        |
| Rmerge               | 0.102              |                        |
| Rpim                 |                    |                        |
| CC1/2 last shell     | 0.38               |                        |
| Wilson B factor (Å²) | 19.5               |                        |

### Refinement

|                      | 6G38               | Re-refinement          |
|----------------------|--------------------|------------------------|
| Rwork / Rfree        | 0.143 / 0.165      | 0.169 / 0.180          |
| Resolution (Å)       | 24.05 - 1.47       | 24.06 - 1.47           |
| Reflections all      | 80839              | 85009                  |
| Reflections for Rfree| 4169, 4.9%         | 4169, 4.9%             |
| Bond lengths rmsd (Å)| 0.012              | 0.016                  |
| Bond angles rmsd (°) | 1.54               | 1.94                   |
| Mean B value (Å²)    | 23                 | 22                     |
| Number of protein atoms | 2595               | 2595                  |
| Mean B value for protein atoms (Å²) | 22               | 21                     |
| Number of water atoms (expected) | 269 (461)          | 269 (461)             |
| Mean B value for water atoms (Å²) | 30               | 30                     |
| Number of ligand/ion atoms | 43             | 43                     |
| Mean B value for ligand/ion atoms (Å²) | 45              | 45                     |
| Clashscore           | 0.38               | 0.38                   |
| Clashscore percentile (100) | -1            | -1                    |
| Rotamer outliers (<1%) | 0.35             | 0.35                   |
| Ramachandran outliers (<0.2%) | 0.00          | 0.00                   |
| Ramachandran favored (>98%) | 98.77        | 98.77                  |
| Residues with bad bonds (<0%) | 0.46        | 0.46                   |
| Residues with bad angles (<0.1%) | 0.46       | 0.46                   |
| MolProbity score     | 0.64               | 0.64                   |

Map cc barchart:
Small molecules with map:

Small molecule 1: '2-(4-AMINO-PYRROLO[2,3-D]PRIMIDIN-7-YL)-5-HYDROXYMETHYL-TETRAHYDRO-FURAN-3,4-DIOL (TBN) A 800 map cc 0.99

Small molecule 2: DIMETHYL SULFOXIDE (DMS) A 801 map cc 0.73
Small molecule 3: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 802 map cc 0.78

Small molecule 4: PHOSPHATE ION (PO4) A 803 map cc 0.85

Credits:

HKL-3000
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Data collection and refinement statistics for project **hepes_6g38** crystal **crystal1**

model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/6g38/structure_mr/build_model_1/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/highres/6g38/structure_mr/build_model_1/hkl_refine_7.pdb

| Data collection                  | 6G38                      | Re-refinement          |
|---------------------------------|---------------------------|------------------------|
| Resolution (Å)                  | 24.05 - 1.43 (1.45 - 1.43) | 56.13 - 1.47           |
| Wavelength (Å)                  | 0.9794                    |                        |
| Space group                     | P212121                   | P212121                |
| a, b, c (Å)                     | 78.56, 78.76, 80.02       | 78.56, 78.76, 80.02    |
| α, β, γ (°)                     | 90, 90, 90                | 90, 90, 90             |
| Completeness (%)                | 99.9 (98.3)               | 100.0 (100.0)          |
| Reflections used                | 92144                     |                        |
| <I> / <Sigma I>                | 8.6 (1.2)                 |                        |
| Redundancy                      | 5.9 (4.2)                 |                        |
| Rmerge                          | 0.102                     |                        |
| Rpim                            |                           |                        |
| CC1/2 last shell                |                           |                        |
| Wilson B factor (Å²)            |                           | 19.5                   |

| Refinement                      |                           |                        |
|---------------------------------|---------------------------|------------------------|
| Rwork / Rfree                   | 0.143 / 0.165             | 0.166 / 0.180          |
| Resolution (Å)                  | 24.05 - 1.47              | 24.06 - 1.47           |
| Reflections all                 | 80839                     | 85009                  |
| Reflections for Rfree           | 4169, 4.9%                | 4169, 4.9%             |
| Bond lengths rmsd (Å)           | 0.012                     | 0.015                  |
| Bond angles rmsd (°)            | 1.54                      | 1.96                   |
| Mean B value (Å²)               | 23                        | 22                     |
| Number of protein atoms         | 2595                      | 2595                   |
| Mean B value for protein atoms (Å²) | 22                  | 21                     |
| Number of water atoms (expected)| 269 (461)                | 269 (461)              |
| Mean B value for water atoms (Å²) | 30                    | 30                     |
| Number of ligand/ion atoms      | 43                        | 43                     |
| Mean B value for ligand/ion atoms (Å²) | 45                    | 44                     |
| Clashscore                      | 0.38                      | 0.96                   |
| Clashscore percentile (100)     | -1                        | -1                     |
| Rotamer outliers (<1%)          | 0.35                      | 0.35                   |
| Ramachandran outliers (<0.2%)   | 0.00                      | 0.00                   |
| Ramachandran favored (>98%)     | 98.77                     | 98.46                  |
| Residues with bad bonds (<0%)   | 0.46                      | 1.07                   |
| Residues with bad angles (<0.1%)| 0.46                      | 1.99                   |
| MolProbity score                | 0.64                      | 0.79                   |

Map cc barchart:
Small molecules with map:

Small molecule 1: '2-(4-AMINO-PYRROLO[2,3-D]PYRIMIDIN-7-YL)-5-HYDROXYMETHYL-TETRAHYDRO-FURAN-3,4-DIOL (TBN) A 800 map cc 0.99

Small molecule 2: DIMETHYL SULFOXIDE (DMS) A 801 map cc 0.80
Small molecule 3: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 802 map cc 0.78

Small molecule 4: PHOSPHATE ION (PO4) A 803 map cc 0.88

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Coot
“Features and Development of Coot”
P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **hepes_4e8r crystal crystal1**

Model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/lowres/4e8r/structure_mr/build_model_1/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/lowres/4e8r/structure_mr/build_model_1/hkl_refine_7.pdb

| Data collection          | 4E8R                                | Re-refinement                      |
|--------------------------|-------------------------------------|------------------------------------|
| Resolution (Å)           | 48.50 - 3.36 (3.45 - 3.36)         | 48.50 - 3.36                       |
| Wavelength (Å)           | 1.4861                              |                                    |
| Space group              | P212121                             | P212121                            |
| a, b, c (Å)              | 90.20, 94.92, 225.71                | 90.20, 94.92, 225.71               |
| α, β, γ (°)              | 90, 90, 90                          | 90, 90, 90                         |
| Completeness (%)         | 97.5 (96.8)                         | 100.0 (100.0)                      |
| Reflections used         | 26102                               |                                    |
| <I> / <Sigma I>          | 15.1 (2.0)                          |                                    |
| Redundancy               | 7.0 (6.7)                           |                                    |
| Rmerge                   |                                     | 0.081                              |
| CC1/2 last shell         |                                     |                                    |

| Refinement               |                                      |                                    |
|--------------------------|-------------------------------------|------------------------------------|
| Rwork / Rfree            | 0.200 / 0.258                       | 0.210 / 0.268                      |
| Resolution (Å)           | 48.50 - 3.36                       | 48.51 - 3.36                       |
| Reflections all          | 26102                               | 27485                              |
| Reflections for Rfree    | 1384, 5.0%                          | 1384, 5.0%                         |
| Bond lengths rmsd (Å)    | 0.007                               | 0.042                              |
| Bond angles rmsd (°)     | 2.39                                | 2.48                               |
| Mean B value (Å²)        | 134                                 | 130                                |
| Number of water atoms    | 26                                  | 26                                 |
| Mean B value for water atoms (Å²) | 80          | 83                                 |
| Number of RNA atoms      | 8412                                | 8412                               |
| Mean B value for RNA atoms (Å²) | 135           | 131                                |
| Number of ligand/ion atoms | 122                             | 122                                |
| Mean B value for ligand/ion atoms (Å²) | 113          | 114                                |
| Clashscore               | 26.75                               | 30.02                              |
| Clashscore percentile (100) | -1                | -1                                 |
| Rotamer outliers (<1%)   | 0.00                                | 0.00                               |
| Ramachandran outliers (<0.2%) | 0.00            | 0.00                               |
| Ramachandran favored (>98%) | 0.00                       | 0.00                               |
| Residues with bad bonds (<0%) | 2.81                      | 2.55                               |
| Residues with bad angles (<0.1%) | 115.56     | 114.29                             |
| MolProbity score         | 3.06                                | 3.11                               |

Map cc barchart:
Small molecules with map:

Small molecule 1: MAGNESIUM ION (MG) A 401 map cc 0.98

Small molecule 2: MAGNESIUM ION (MG) A 402 map cc 0.95
Small molecule 3: MAGNESIUM ION (MG) A 403 map cc 0.94

Small molecule 4: MAGNESIUM ION (MG) A 404 map cc 0.98

Small molecule 5: MAGNESIUM ION (MG) A 405 map cc 0.89

Small molecule 6: MAGNESIUM ION (MG) A 406 map cc 0.97
Small molecule 7: MAGNESIUM ION (Mg) A 407 map cc 0.95

Small molecule 8: MAGNESIUM ION (Mg) A 408 map cc 0.97

Small molecule 9: MAGNESIUM ION (Mg) A 409 map cc 0.88

Small molecule 10: MAGNESIUM ION (Mg) A 410 map cc 0.73
Small molecule 11: MAGNESIUM ION (MG) A 411 map cc 0.44

Small molecule 12: MAGNESIUM ION (MG) A 412 map cc 0.94

Small molecule 13: MAGNESIUM ION (MG) A 413 map cc 0.99

Small molecule 14: MAGNESIUM ION (MG) A 414 map cc 0.98
Small molecule 15: MAGNESIUM ION (MG) A 415 map cc 1.00

Small molecule 16: MAGNESIUM ION (MG) A 416 map cc 0.26

Small molecule 17: MAGNESIUM ION (MG) A 417 map cc 0.96

Small molecule 18: MAGNESIUM ION (MG) A 418 map cc 0.99
Small molecule 19: MAGNESIUM ION (MG) A 419 map cc 0.98

Small molecule 20: MAGNESIUM ION (MG) A 420 map cc 1.00

Small molecule 21: MAGNESIUM ION (MG) A 421 map cc 0.99

Small molecule 22: MAGNESIUM ION (MG) A 422 map cc 0.14
Small molecule 23: MAGNESIUM ION (MG) A 423 map cc 0.98

Small molecule 24: CESIUM ION (CS) A 424 map cc 0.93

Small molecule 25: CESIUM ION (CS) A 425 map cc 0.99

Small molecule 26: CESIUM ION (CS) A 426 map cc 0.95
Small molecule 27: CESIUM ION (CS) A 427 map cc 0.95

Small molecule 28: CESIUM ION (CS) A 428 map cc 0.81

Small molecule 29: CESIUM ION (CS) A 429 map cc 1.00

Small molecule 30: CESIUM ION (CS) A 430 map cc 1.00
Small molecule 31: CESIUM ION (CS) A 431 map cc 1.00

Small molecule 32: CESIUM ION (CS) A 432 map cc 1.00

Small molecule 33: CESIUM ION (CS) A 433 map cc 0.99

Small molecule 34: CESIUM ION (CS) A 434 map cc 1.00
Small molecule 35: CESIUM ION (CS) A 435 map cc 0.99

Small molecule 36: CESIUM ION (CS) A 436 map cc 0.98

Small molecule 37: CESIUM ION (CS) A 437 map cc 1.00

Small molecule 38: CESIUM ION (CS) A 438 map cc 0.92
Small molecule 39: CESIUM ION (CS) A 439 map cc 1.00

Small molecule 40: CESIUM ION (CS) A 440 map cc 0.97

Small molecule 41: CESIUM ION (CS) A 441 map cc 0.98

Small molecule 42: CESIUM ION (CS) A 442 map cc 1.00
Small molecule 43: CESIUM ION (CS) A 443 map cc 1.00

Small molecule 44: CESIUM ION (CS) A 444 map cc 0.99

Small molecule 45: CESIUM ION (CS) A 445 map cc 0.67

Small molecule 46: CESIUM ION (CS) A 446 map cc 1.00
Small molecule 47: CESIUM ION (CS) A 447 map cc 0.97

Small molecule 48: CESIUM ION (CS) A 448 map cc 0.99

Small molecule 49: CESIUM ION (CS) A 449 map cc 0.81

Small molecule 50: CESIUM ION (CS) A 450 map cc 0.90
Small molecule 51: CESIUM ION (CS) A 451 map cc 0.87

Small molecule 52: CESIUM ION (CS) A 452 map cc 1.00

Small molecule 53: CESIUM ION (CS) A 453 map cc 1.00

Small molecule 54: CESIUM ION (CS) A 454 map cc 0.66
Small molecule 55: CESIUM ION (CS) A 455 map cc 1.00

Small molecule 56: CESIUM ION (CS) A 456 map cc 1.00

Small molecule 57: CESIUM ION (CS) A 457 map cc 0.92

Small molecule 58: CESIUM ION (CS) A 458 map cc 0.98
Small molecule 59: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 459 map cc 0.86

Small molecule 60: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 460 map cc 0.85

Small molecule 61: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 461 map cc 0.83

Small molecule 62: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 462 map cc 0.79
Small molecule 63: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 463 map cc 0.99

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Acta Cryst. D66, 486-501 (2010)
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|-------------------------|-----------------------|----------------------|
| Resolution (Å)          | 48.50 - 3.36 (3.45 - 3.36) | 48.50 - 3.36          |
| Wavelength (Å)          | 1.4861                |                      |
| Space group             | P212121               | P212121              |
| a, b, c (Å)             | 90.20, 94.92, 225.71  | 90.20, 94.92, 225.71 |
| α, β, γ (°)             | 90, 90, 90            | 90, 90, 90           |
| Completeness (%)        | 97.5 (96.8)           | 100.0 (100.0)        |
| Reflections used        | 26102                 |                      |
| <I> / <Sigma I>         | 15.1 (2.0)            |                      |
| Redundancy              | 7.0 (6.7)             |                      |
| Rmerge                  |                      | 0.081                |
| CC1/2 last shell        |                      |                      |

| Refinement              |                      |                      |
|-------------------------|-----------------------|----------------------|
| Rwork / Rfree           | 0.200 / 0.258         | 0.199 / 0.260        |
| Resolution (Å)          | 48.50 - 3.36          | 48.51 - 3.36         |
| Reflections all         | 26102                 | 27485                |
| Reflections for Rfree   | 1384, 5.0%            | 1384, 5.0%           |
| Bond lengths rmsd (Å)   | 0.007                 | 0.009                |
| Bond angles rmsd (°)    | 2.39                  | 1.80                 |
| Mean B value (Å²)       | 134                   | 133                  |
| Number of water atoms   | 26                    | 26                   |
| Mean B value for water atoms (Å²) | 80            | 80                   |
| Number of RNA atoms     | 8412                  | 8412                 |
| Mean B value for RNA atoms (Å²) | 135              | 133                  |
| Number of ligand/ion atoms | 122              | 122                  |
| Mean B value for ligand/ion atoms (Å²) | 113            | 115                  |
| Clashscore              | 26.75                 | 7.41                 |
| Clashscore percentile (100) | -1              | -1                   |
| Rotamer outliers (<1%)  | 0.00                  | 0.00                 |
| Ramachandran outliers (<0.2%) | 0.00     | 0.00                 |
| Ramachandran favored (>98%) | 0.00           | 0.00                 |
| Residues with bad bonds (<0%) | 2.81          | 3.57                 |
| Residues with bad angles (<0.1%) | 115.56    | 56.89                |
| MolProbity score        | 3.06                  | 2.56                 |

Map cc barchart:
Small molecules with map:

Small molecule 1: MAGNESIUM ION (MG) A 401 map cc 0.99

Small molecule 2: MAGNESIUM ION (MG) A 402 map cc 1.00
Small molecule 3: MAGNESIUM ION (MG) A 403 map cc 0.98

Small molecule 4: MAGNESIUM ION (MG) A 404 map cc 0.76

Small molecule 5: MAGNESIUM ION (MG) A 405 map cc 0.75

Small molecule 6: MAGNESIUM ION (MG) A 406 map cc 0.95
Small molecule 7: MAGNESIUM ION (MG) A 407 map cc 1.00

Small molecule 8: MAGNESIUM ION (MG) A 408 map cc 0.99

Small molecule 9: MAGNESIUM ION (MG) A 409 map cc 0.74

Small molecule 10: MAGNESIUM ION (MG) A 410 map cc 1.00
Small molecule 11: MAGNESIUM ION (MG) A 411 map cc 0.31

Small molecule 12: MAGNESIUM ION (MG) A 412 map cc 0.92

Small molecule 13: MAGNESIUM ION (MG) A 413 map cc 0.98

Small molecule 14: MAGNESIUM ION (MG) A 414 map cc 0.99
Small molecule 15: MAGNESIUM ION (MG) A 415 map cc 1.00

Small molecule 16: MAGNESIUM ION (MG) A 416 map cc 0.54

Small molecule 17: MAGNESIUM ION (MG) A 417 map cc 0.91

Small molecule 18: MAGNESIUM ION (MG) A 418 map cc 1.00
Small molecule 19: MAGNESIUM ION (MG) A 419 map cc 0.99

Small molecule 20: MAGNESIUM ION (MG) A 420 map cc 1.00

Small molecule 21: MAGNESIUM ION (MG) A 421 map cc 0.95

Small molecule 22: MAGNESIUM ION (MG) A 422 map cc 0.98
Small molecule 23: MAGNESIUM ION (MG) A 423 map cc 0.89

Small molecule 24: CESIUM ION (CS) A 424 map cc 0.93

Small molecule 25: CESIUM ION (CS) A 425 map cc 0.97

Small molecule 26: CESIUM ION (CS) A 426 map cc 0.88
Small molecule 27: CESIUM ION (CS) A 427 map cc 0.96

Small molecule 28: CESIUM ION (CS) A 428 map cc 0.86

Small molecule 29: CESIUM ION (CS) A 429 map cc 1.00

Small molecule 30: CESIUM ION (CS) A 430 map cc 1.00
Small molecule 31: CESIUM ION (CS) A 431 map cc 1.00

Small molecule 32: CESIUM ION (CS) A 432 map cc 1.00

Small molecule 33: CESIUM ION (CS) A 433 map cc 0.98

Small molecule 34: CESIUM ION (CS) A 434 map cc 0.99
Small molecule 35: CESIUM ION (CS) A 435 map cc 0.58

Small molecule 36: CESIUM ION (CS) A 436 map cc 0.97

Small molecule 37: CESIUM ION (CS) A 437 map cc 1.00

Small molecule 38: CESIUM ION (CS) A 438 map cc 0.89
Small molecule 39: CESIUM ION (CS) A 439 map cc 0.99

Small molecule 40: CESIUM ION (CS) A 440 map cc 0.72

Small molecule 41: CESIUM ION (CS) A 441 map cc 1.00

Small molecule 42: CESIUM ION (CS) A 442 map cc 0.92
Small molecule 43: CESIUM ION (CS) A 443 map cc 0.92

Small molecule 44: CESIUM ION (CS) A 444 map cc 1.00

Small molecule 45: CESIUM ION (CS) A 445 map cc 0.96

Small molecule 46: CESIUM ION (CS) A 446 map cc 1.00
Small molecule 47: CESIUM ION (CS) A 447 map cc 0.96

Small molecule 48: CESIUM ION (CS) A 448 map cc 0.97

Small molecule 49: CESIUM ION (CS) A 449 map cc 0.90

Small molecule 50: CESIUM ION (CS) A 450 map cc 0.82
Small molecule 51: CESIUM ION (CS) A 451 map cc 0.49

Small molecule 52: CESIUM ION (CS) A 452 map cc 0.77

Small molecule 53: CESIUM ION (CS) A 453 map cc 0.94

Small molecule 54: CESIUM ION (CS) A 454 map cc 0.49
Small molecule 55: CESIUM ION (CS) A 455 map cc 1.00

Small molecule 56: CESIUM ION (CS) A 456 map cc 1.00

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Small molecule 61: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 461 map cc 0.86

Small molecule 62: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 462 map cc 0.82
Small molecule 63: 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONICACID (EPE) A 463 map cc 1.00

Credits:

HKL-3000
"Processing of X-ray Diffraction Data Collected in Oscillation Mode"
Z.Otwinowski, W.Minor
Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p307-326 (1997)
"HKL-3000: the integration of data reduction and structure solution - from diffraction images to an initial model in minutes"
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"Overview of the CCP4 suite and current developments"
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"REFMAC5 for the refinement of macromolecular crystal structures"
G.N.Murshudov, P.Skubak, A.A.Lebedev, N.S.Pannu, R.A.Steiner, R.A.Nicholls, M.D.Winn, F.Long and A.A.Vagin
Acta Cryst. D67, 355-367 (2011)

Coot
"Features and Development of Coot"
P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project `mes_4z91` crystal `crystal1`

| Model | `model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/lowres/4z91/structure_mr/build_model_1/hkl_import.pdb` vs `model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/lowres/4z91/structure_mr/build_model_1/hkl_refine_3.pdb` |

| **Data collection** | 4Z91 | Re-refinement |
|---------------------|-------|---------------|
| Resolution (Å)      | 40.01 - 3.39 (3.46 - 3.39) | 40.01 - 3.39 |
| Wavelength (Å)      | 0.9199 | P21 |
| Space group         | P21 | P21 |
| a, b, c (Å)         | 105.76, 267.60, 111.37 | 105.76, 267.60, 111.37 |
| a, β, γ (°)         | 90, 107.80, 90 | 90, 107.80, 90 |
| Completeness (%)    | 98.1 (91.6) | 100.0 (100.0) |
| Reflections used    | 156498 | 79300 |
| <I> / <Sigma I>     | 12.2 | 7.0 (6.6) |
| Redundancy          | 1.43 | 1.96 |
| Rmerge              | 0.146 | 0.017 |
| Rpim                | 0.146 | 0.017 |
| CC1/2 last shell    | 25270 | 25270 |

| Refinement | 4Z91 | Re-refinement |
|-------------|------|---------------|
| Rwork / Rfree | 0.192 / 0.247 | 0.207 / 0.256 |
| Resolution (Å) | 34.89 - 3.39 | 40.01 - 3.39 |
| Reflections all | 156498 | 79300 |
| Reflections for Rfree | 3986, 2.5% | 2018, 2.5% |
| Bond lengths rmsd (Å) | 0.11 | 0.011 |
| Bond angles rmsd (°) | 1.43 | 1.96 |
| Mean B value (Å²) | 116 | 122 |
| Number of protein atoms | 116 | 122 |
| Mean B value for protein atoms (Å²) | 25270 | 25270 |
| Number of water atoms | 81 | 81 |
| Mean B value for water atoms (Å²) | 91 | 90 |
| Number of ligand/ion atoms | 180 | 180 |
| Mean B value for ligand/ion atoms (Å²) | 160 | 172 |
| Clashscore | 13.52 | 13.50 |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 2.27 | 2.27 |
| Ramachandran outliers (<0.2%) | 0.33 | 0.33 |
| Ramachandran favored (>98%) | 92.02 | 92.02 |
| Residues with bad bonds (<0%) | 0.00 | 0.03 |
| Residues with bad angles (<0.1%) | 0.00 | 0.03 |
| MolProbity score | 2.40 | 2.40 |

Map cc barchart:
Small molecules with map:

Small molecule 1: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) A 401 map cc 0.95

Small molecule 2: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 402 map cc 0.96
Small molecule 3: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 401 map cc 0.73

Small molecule 4: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) C 401 map cc 0.78

Small molecule 5: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) D 401 map cc 0.88

Small molecule 6: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) E 401 map cc 0.98
Small molecule 7: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) E 402 map cc 0.81

Small molecule 8: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) F 401 map cc 0.99

Small molecule 9: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) F 402 map cc 0.90

Small molecule 10: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) G 401 map cc 0.94
Small molecule 11: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) H 401 map cc 0.96

Small molecule 12: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) I 401 map cc 0.72

Small molecule 13: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) J 401 map cc 0.97

Small molecule 14: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) J 402 map cc 0.84
Credits:

HKL-3000
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Z.Otwinowski, W.Minor
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Coot
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P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **mes_4z91** crystal **crystal1**

model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/lowres/4z91/structure_mr/build_model_1/hkl_import.pdb vs
model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/lowres/4z91/structure_mr/build_model_1/hkl_refine_4.pdb

### Data collection

| Resolution (Å)                     | 4Z91         | Re-refinement |
|-----------------------------------|--------------|---------------|
| Wavelength (Å)                    | 40.01 - 3.39 | 40.01 - 3.39  |
| Space group                       | P21          | P21           |
| a, b, c (Å)                       | 105.76, 267.60, 111.37 |
| a, b, c (Å)                       | 90, 107.80, 90 |
| Completeness (%)                  | 98.1 (91.6)  | 100.0 (100.0) |
| Reflections used                  | 156498       |               |
| <I> / <Sigma I>                   | 12.2         |               |
| Redundancy                        | 7.0 (6.6)    |               |
| Rmerge                            | 0.146        |               |
| Rpim                              |              |               |
| CC1/2 last shell                  |              |               |

### Refinement

| Rwork / Rfree                     | 0.192 / 0.247 | 0.186 / 0.251 |
| Resolution (Å)                    | 34.89 - 3.39  | 40.01 - 3.39  |
| Reflections all                   | 156498        | 79300         |
| Reflections for Rfree             | 3986, 2.5%    | 2018, 2.5%    |
| Bond lengths rmsd (Å)             | 0.011         | 0.007         |
| Bond angles rmsd (°)              | 1.43          | 1.65          |
| Mean B value (Å²)                 | 116           | 127           |
| Number of protein atoms           | 25270         | 25270         |
| Mean B value for protein atoms (Å²)| 116           | 127           |
| Number of water atoms             | 81            | 81            |
| Mean B value for water atoms (Å²)  | 91            | 89            |
| Number of ligand/ion atoms        | 180           | 180           |
| Mean B value for ligand/ion atoms (Å²)| 160           | 180           |
| Clashscore                        | 13.52         | 7.78          |
| Clashscore percentile (100)       | -1            | -1            |
| Rotamer outliers (<1%)            | 2.27          | 4.95          |
| Ramachandran outliers (<0.2%)     | 0.33          | 2.44          |
| Ramachandran favored (>98%)       | 92.02         | 87.10         |
| Residues with bad bonds (<0%)     | 0.00          | 0.32          |
| Residues with bad angles (<0.1%)  | 0.00          | 1.26          |
| MolProbity score                  | 2.40          | 2.57          |

### Map cc barchart:
Small molecules with map:

Small molecule 1: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) A 401 map cc 0.98

Small molecule 2: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 402 map cc 0.93
Small molecule 3: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) B 401 map cc 0.78

Small molecule 4: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) C 401 map cc 0.70

Small molecule 5: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) D 401 map cc 0.96

Small molecule 6: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) E 401 map cc 0.97
Small molecule 7: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) E 402 map cc 0.89

Small molecule 8: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) F 401 map cc 0.97

Small molecule 9: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) F 402 map cc 0.89

Small molecule 10: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) G 401 map cc 0.84
Small molecule 11: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) H 401 map cc 0.94

Small molecule 12: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) I 401 map cc 0.76

Small molecule 13: (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (4LE) J 401 map cc 0.94

Small molecule 14: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) J 402 map cc 0.78
Credits:

HKL-3000
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Reffmac5
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Coot
"Features and Development of Coot"
P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **mes_3e9f crystal crystal1**

model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/3e9f/structure_mr/build_model_1/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/3e9f/structure_mr/build_model_1/hkl_refine_3.pdb

### Data collection

|             | 3E9F          | Re-refinement |
|-------------|---------------|---------------|
| Resolution (Å) | 50.00 - 1.80 (1.86 - 1.80) | 25.81 - 1.80 |
| Wavelength (Å) | 1.0000       |               |
| Space group   | C2221         | C2221         |
| a, b, c (Å)   | 34.62, 130.34, 56.21 | 34.62, 130.34, 56.21 |
| α, β, γ (°)   | 90, 90, 90    | 90, 90, 90    |
| Completeness (%) | 99.3          | 100.0 (100.0) |
| Reflections used | 12156        |               |
| <I> / <Sigma I> | 6.5 (5.8)    |               |
| Redundancy    |               |               |
| Rmerge        | 0.110         |               |
| Rpim          |               |               |

### Refinement

|             | 3E9F          | Re-refinement |
|-------------|---------------|---------------|
| Rwork / Rfree | 0.188 / 0.217 | 0.182 / 0.174 |
| Resolution (Å) | 25.81 - 1.80 | 25.81 - 1.80 |
| Reflections all | 12141       | 12142         |
| Reflections for Rfree | 610, 5.0%    | 580, 4.8%     |
| Bond lengths rmsd (Å) | 0.015      | 0.018         |
| Bond angles rmsd (°) | 1.57       | 1.87          |
| Mean B value (Å²) | 26          | 28            |
| Number of protein atoms | 818        | 818           |
| Mean B value for protein atoms (Å²) | 24      | 27            |
| Number of water atoms (expected) | 123 (123)  | 123 (123)     |
| Mean B value for water atoms (Å²) | 38       | 40            |
| Number of ligand/ion atoms | 12      | 12            |
| Mean B value for ligand/ion atoms (Å²) | 37    | 38            |
| Clashscore    | 3.66          | 3.65          |
| Clashscore percentile (100) | -1       | -1            |
| Rotamer outliers (<1%) | 2.33   | 2.33          |
| Ramachandran outliers (<0.2%) | 0.00  | 0.00          |
| Ramachandran favored (>98%) | 97.89 | 97.89         |
| Residues with bad bonds (<0%) | 1.01   | 2.02          |
| Residues with bad angles (<0.1%) | 0.00  | 0.00          |
| MolProbity score | 1.46   | 1.46          |

### Map cc barchart:

Small molecules with map:
Small molecule 1: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 122 map cc 0.97

Credits:

HKL-3000
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Data collection and refinement statistics for project **mes_3e9f crystal crystal1**

|                | 3E9F          | Re-refinement |
|----------------|---------------|---------------|
| Resolution (Å) | 50.00 - 1.80  | 25.81 - 1.80  |
| Wavelength (Å) | 1.0000        |               |
| Space group    | C2221         | C2221         |
| a, b, c (Å)    | 34.62, 130.34, 56.21 | 34.62, 130.34, 56.21 |
| a, β, γ (°)    | 90, 90, 90    | 90, 90, 90    |
| Completeness (%) | 99.3         | 100.0 (100.0) |
| Reflections used | 12156         |               |
| <I> / <Sigma I> |               |               |
| Redundancy     | 6.5 (5.8)     |               |
| Rmerge         | 0.110         |               |
| Wilson B factor (Å²) | 22.0 |        |

**Refinement**

|                | 0.188 / 0.217 | 0.175 / 0.193 |
|----------------|---------------|---------------|
| Resolution (Å) | 25.81 - 1.80  | 25.81 - 1.80  |
| Reflections all | 12141         | 12142         |
| Reflections for Rfree | 610, 5.0% | 580, 4.8% |
| Bond lengths rmsd (Å) | 0.015        | 0.012         |
| Bond angles rmsd (°)  | 1.57          | 1.74          |
| Mean B value (Å²)   | 26            | 28            |
| Number of protein atoms | 818         | 818            |
| Mean B value for protein atoms (Å²) | 24        | 26             |
| Number of water atoms (expected) | 123 (123) | 123 (123) |
| Mean B value for water atoms (Å²) | 38        | 39             |
| Number of ligand/ion atoms | 12         | 12             |
| Mean B value for ligand/ion atoms (Å²) | 37       | 38             |
| Clashscore         | 3.66          | 3.65          |
| Clashscore percentile (100) | -1            | -1            |
| Rotamer outliers (<1%) | 2.33        | 0.00          |
| Ramachandran outliers (<0.2%) | 0.00        | 0.00          |
| Ramachandran favored (>98%) | 97.89       | 100.00        |
| Residues with bad bonds (<0%) | 1.01         | 2.02          |
| Residues with bad angles (<0.1%) | 0.00        | 1.01          |
| MolProbity score   | 1.46          | 1.16          |

**Map cc barchart:**

```
Chain A

F A L G R C L A F H G L M Y E A K I L K I W O P S S K M Y T S I P N K E I K P Q K L G E
D E S I F E D I N G K C F F I H V Q W H S S W D E W V O V D R I B A Y N E N I A M K R

Chain A - small molecules: MES

Chain A - water molecules

Legend
> 0.95 > 0.9 > 0.8 > 0.7 > 0.6 <= 0.6

Small molecules with map:
Small molecule 1: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 122 map cc 0.97

Credits:

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P.Emsley, B.Lohkamp, W.Scott, and K.Cowtan
Acta Cryst. D66, 486-501 (2010)
Data collection and refinement statistics for project **mes_1mos** crystal **crystal1**

| Model 1 | Model 2 |
|---------|---------|
| /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1mos/structure_mr/build_model_1/hkl_import.pdb | /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1mos/structure_mr/build_model_1/hkl_refine_3.pdb |

### Data collection

|                      | 1MOS                  | Re-refinement |
|----------------------|-----------------------|---------------|
| Resolution (Å)       | 25.00 - 2.00 (2.03 - 2.00) | 24.67 - 2.00  |
| Wavelength (Å)       |                       |               |
| Space group          | H32                   | R32           |
| a, b, c (Å)          | 143.90, 143.90, 172.80 | 143.90, 143.90, 172.80 |
| α, β, γ (°)          | 90, 90, 120           | 90, 90, 120   |
| Completeness (%)     | 98.7 (95.7)           | 100.0 (100.0) |
| Reflections used     | 45840                 |               |
| <I> / <Sigma I>      | 3.6 (3.6)             |               |
| Redundancy           | 9.1 (2.6)             |               |
| Rmerge               | 0.058                 |               |
| Wilson B factor (Å²) | 27.4                  |               |

### Refinement

|                      | 1MOS                  | Re-refinement |
|----------------------|-----------------------|---------------|
| Rwork / Rfree        | / 0.287               | 0.205 / 0.245 |
| Resolution (Å)       | 12.00 - 2.00          | 24.67 - 2.00  |
| Reflections all      | 45626                 | 45840         |
| Reflections for Rfree| , 5.0%                | 2338, 5.1%    |
| Bond lengths rmsd (Å)| 0.015                 | 0.013         |
| Bond angles rmsd (°) |                       | 1.79          |
| Mean B value (Å²)    | 37                    | 39            |
| Number of protein atoms | 2824                 | 2824          |
| Mean B value for protein atoms (Å²) | 37 | 39 |
| Number of water atoms (expected) | 180 (315) | 180 (315) |
| Mean B value for water atoms (Å²) | 44 | 43 |
| Number of ligand/ion atoms | 44 | 44 |
| Mean B value for ligand/ion atoms (Å²) | 42 | 42 |
| Clashscore           | 7.83                  | 3.83          |
| Clashscore percentile (100) | -1                  | -1            |
| Rotamer outliers (<1%) | 3.28                 | 1.64          |
| Ramachandran outliers (<0.2%) | 0.00                 | 0.00          |
| Ramachandran favored (>98%) | 98.36                | 98.90         |
| Residues with bad bonds (<0%) | 2.45                 | 0.82          |
| Residues with bad angles (<0.1%) | 8.99                 | 2.18          |
| MolProbity score     | 1.82                  | 1.33          |

**Map cc barchart:**
Small molecules with map:

Small molecule 1: SULFATE ION (SO4) A 611 map cc 0.85

Small molecule 2: SULFATE ION (SO4) A 612 map cc 0.93
Small molecule 3: SULFATE ION (SO4) A 613 map cc 0.94

Small molecule 4: SODIUM ION (NA) A 614 map cc 0.95

Small molecule 5: 2-DEOXY-2-AMINO GLUCITOL-6-PHOSPHATE (AGP) A 609 map cc 0.98

Small molecule 6: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 610 map cc 0.97
Credits:

HKL-3000
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Model: `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1mos/structure_mr/build_model_1/hkl_import.pdb` vs model: `/home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1mos/structure_mr/build_model_1/hkl_refine_4.pdb`

### Data collection

|                      | 1MOS                   | Re-refinement          |
|----------------------|------------------------|------------------------|
| Resolution (Å)       | 25.00 - 2.00 (2.03 - 2.00) | 24.67 - 2.00           |
| Wavelength (Å)       |                        |                        |
| Space group          | H32                    | R32                    |
| a, b, c (Å)          | 143.90, 143.90, 172.80 | 143.90, 143.90, 172.80 |
| α, β, γ (°)          | 90, 90, 120            | 90, 90, 120            |
| Completeness (%)     | 98.7 (95.7)            | 100.0 (100.0)          |
| Reflections used     | 45,840                 |                        |
| <I> / <Sigma I>     | 3.6 (3.6)              |                        |
| Redundancy           | 9.1 (2.6)              |                        |
| Rmerge               | 0.058                  |                        |
| Wilson B factor (Å²) | 27.4                   |                        |

### Refinement

|                      | 1MOS                   | Re-refinement          |
|----------------------|------------------------|------------------------|
| Rwork / Rfree        | / 0.287                | 0.205 / 0.246          |
| Resolution (Å)       | 12.00 - 2.00           | 24.67 - 2.00           |
| Reflections all      | 45,626                 | 45,840                 |
| Reflections for Rfree| .5.0%                  | 2338, 5.1%             |
| Bond lengths rmsd (Å)| 0.015                  | 0.013                  |
| Bond angles rmsd (°) |                        | 1.79                   |
| Mean B value (Å²)    | 37                     | 39                     |
| Number of protein atoms | 2824                  | 2824                  |
| Mean B value for protein atoms (Å²) | 37                  | 39                  |
| Number of water atoms (expected) | 180 (315)              | 180 (315)             |
| Mean B value for water atoms (Å²) | 44                    | 43                    |
| Number of ligand/ion atoms | 44                   | 44                    |
| Mean B value for ligand/ion atoms (Å²) | 42                    | 42                    |
| Clashscore           | 7.83                   | 3.13                   |
| Clashscore percentile (100) | -1                    | -1                    |
| Rotamer outliers (<1%) | 3.28                   | 1.64                   |
| Ramachandran outliers (<0.2%) | 0.00                   | 0.00                   |
| Ramachandran favored (>98%) | 98.36                  | 98.90                  |
| Residues with bad bonds (<0%) | 2.45                   | 0.54                   |
| Residues with bad angles (<0.1%) | 8.99                   | 1.63                   |
| MolProbity score     | 1.82                   | 1.27                   |

### Map cc barchart:
Small molecules with map:

Small molecule 1: SULFATE ION (SO₄) A 611 map cc 0.85

Small molecule 2: SULFATE ION (SO₄) A 612 map cc 0.93
Small molecule 3: SULFATE ION (SO4) A 613 map cc 0.94

Small molecule 4: SODIUM ION (NA) A 614 map cc 0.95

Small molecule 5: 2-DEOXY-2-AMINO GLUCITOL-6-PHOSPHATE (AGP) A 609 map cc 0.98

Small molecule 6: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 610 map cc 0.97
Credits:

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Data collection and refinement statistics for project **mes_1moq** crystal **crystal1**

Model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1moq/structure_mr/build_model_1/hkl_import.pdb vs model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1moq/structure_mr/build_model_1/hkl_refine_3.pdb

| Data collection         | 1MOQ                  | Re-refinement       |
|-------------------------|-----------------------|---------------------|
| Resolution (Å)          | 30.00 - 1.57 (1.60 - 1.57) | 28.17 - 1.57        |
| Wavelength (Å)          |                       |                     |
| Space group             | H32                   | R32                 |
| a, b, c (Å)             | 143.70, 143.70, 173.60 | 143.70, 143.70, 173.60 |
| α, β, γ (°)             | 90, 90, 120           | 90, 90, 120         |
| Completeness (%)        | 99.5 (96.2)           | 100.0 (100.0)       |
| Reflections used        | 95543                 |                     |
| <I> / <Sigma I>         | 39.2 (5.7)            |                     |
| Redundancy              | 6.5 (3.3)             |                     |
| Rmerge                   | 0.040                 |                     |
| Wilson B factor (Å²)    | 18.0                  |                     |

| Refinement              |                      |                     |
| Rwork / Rfree           | 0.185 / 0.133        | 0.133 / 0.140       |
| Resolution (Å)          | 10.00 - 1.57         | 28.19 - 2.50        |
| Reflections all         | 94943                | 23962               |
| Reflections for Rfree   | %                     | 1180, 4.9%          |
| Bond lengths rmsd (Å)   | 0.014                | 0.019               |
| Bond angles rmsd (°)    |                      | 2.65                |
| Mean B value (Å²)       | 25                   | 24                  |
| Mean B value for protein atoms (Å²) | 22 | 22 |
| Number of protein atoms | 2825                 | 2825                |
| Mean B value for water atoms (Å²) | 40 | 37 |
| Number of water atoms (expected) | 416 (445) | 416 (445) |
| Mean B value for saccharide atoms | 16 | 16 |
| Number of saccharide atoms | 14 | 13 |
| Mean B value for ligand/ion atoms (Å²) | 38 | 34 |
| Clashscore              | 5.71                 | 5.36                |
| Clashscore percentile (100) | -1                  | -1                  |
| Rotamer outliers (<1%)  | 0.98                 | 0.98                |
| Ramachandran outliers (<0.2%) | 0.00            | 0.00                |
| Ramachandran favored (>98%) | 98.35            | 98.35               |
| Residues with bad bonds (<0%) | 0.55            | 0.27                |
| Residues with bad angles (<0.1%) | 4.78            | 4.37                |
| MolProbity score        | 1.31                 | 1.29                |

**Map cc barchart:**
Small molecules with map:

Small molecule 1: GLUCOSAMINE 6-PHOSPHATE (GLP) A 609 map cc 0.99

Small molecule 2: SULFATE ION (SO4) A 612 map cc 0.97
Small molecule 3: SULFATE ION (SO4) A 613 map cc 0.86

Small molecule 4: SULFATE ION (SO4) A 614 map cc 0.98

Small molecule 5: SULFATE ION (SO4) A 615 map cc 0.94

Small molecule 6: SULFATE ION (SO4) A 616 map cc 0.97
Small molecule 7: SODIUM ION (NA) A 617 map cc 0.91

Small molecule 8: 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (MES) A 610 map cc 0.99

Small molecule 9: (4R)-2-METHYL-PENTANE-2,4-DIOL (MRD) A 611 map cc 0.98

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model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1moq/structure_mr/build_model_1/hkl_import.pdb
model /home/asia/epe-like-validation/RESULTS/HKL_rerefine/flat/1moq/structure_mr/build_model_1/hkl_refine_4.pdb

| Data collection | 1MOQ | Re-refinement |
|-----------------|------|---------------|
| Resolution (Å)  | 30.00 - 1.57 (1.60 - 1.57) | 28.17 - 1.57 |
| Wavelength (Å)  | 143.70, 143.70, 173.60 | 143.70, 143.70, 173.60 |
| Space group     | H32  | R32           |
| a, b, c (Å)     | 90, 90, 120 | 90, 90, 120 |
| a, β, γ (°)     | 99.5 (96.2) | 100.0 (100.0) |
| Completess (%)  | 95543 |               |
| <I> / <Sigma I> | 39.2 (5.7) |               |
| Redundancy      | 6.5 (3.3) |               |
| Wilson B factor (Å²) | 18.0 |               |

| Refinement       | 1MOQ | Re-refinement |
|------------------|------|---------------|
| Rwork / Rfree    | 0.185 / 0.121 / 0.156 |               |
| Resolution (Å)   | 10.00 - 1.57 | 28.19 - 2.50 |
| Reflections all  | 94943 | 23962         |
| Reflections for Rfree | % | 1180, 4.9% |
| Bond lengths rmsd (Å) | 0.014 | 0.014 |
| Bond angles rmsd (°) | 1.83 |               |
| Mean B value (Å²) | 25   | 24            |
| Number of protein atoms | 2825 | 2825         |
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| Mean B value for water atoms (Å²) | 40 | 36 |
| Number of saccharide atoms | 16 | 16 |
| Mean B value for saccharide atoms (Å²) | 14 | 14 |
| Number of ligand/ion atoms | 46 | 46 |
| Mean B value for ligand/ion atoms (Å²) | 38 | 35 |
| Clashscore       | 5.71 | 3.80          |
| Clashscore percentile (100) | -1 | -1 |
| Rotamer outliers (<1%) | 0.98 | 1.30 |
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| Ramachandran favored (>98%) | 98.35 | 98.63 |
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