The data file – 3nir.mtz do not have a r-free-flags or the flags is not suitable for refinement.

res 1

ATHR bad hydrogen geometry on N, not pyramidal, H3 distance 1.19 – maybe HBond

to the O Res35, BIG

ATHR positive density on CB, CG2 while there is no density on CB of altloc B BIG

BTHR three hydrogen connect to N floating, CA-C-O angle 109 (120)

res 2

ATHR negative density around OG1

BTHR HA too close to CB, N-H too long 1.39

BTHR O-C-N angle 131 (123), H stick out the peptide plane

res 3 H stick out the peptide plane for both altlocs A and B

res 4 lots of positive and negative density around SG

res 5 red and green density on opposite sides of O – possible HBond to res 20

res 6 HG point to negative density, following green one can lead to a hydrogen bond with symmetry copy

res 7 BILE HA floating, HB to close to CB (0.27 A) BIG

BILE HG23 clash with water 3017B3

BILE CG1 has a green density BIG

BILE CG2 methyl group bad geometry, CG2-HG21 longer than the ideal value

res 8

AVAL positive density around CG1, CG2, consider add a conformer, O-C-N angle 130

BVAL HB floating, negative density around CG1, CG2, O-C-N angle 112 (123)

O point to negative density for both altlocs

res 10 ARG side chain can add a conformer, non-spherical density along arginine out-plane-direction with red and green on opposite end, H stick out the peptide plane

res 11 clash with ligand 2002 EOH

res 12 positive density around C, O covering both altlocs –what can be missing there?

N-O not in the peptide plane

res 13 APHE HA floating, O-C-N angle 129

BPHE HA floating and hydrogen connect to ring floating

BPHE O-C-N angle 111.6, N-O not in the peptide plane

Hydron connect to the ring are not in plane

res 14 ASN side chain, ND2, OD1 have hydrogen bond with water 3018,3019,3014,3047A, push to away negative density

res 15 mess positive density around main chain, green density on one side of main chain – add altloc?

res 16 lots of positive and negative density around SG

res 17 just some noise

res 18 HB2 clash with res 19 BPRO HD3 (but its 1.8 A)

res 19 HA altloc B too close to CB – (angle to the ring not OK) BIG

res 21 THR O has red and green densities on opposite sides of the C=O bond (there is also possible HBond to HH11 of residue 17)

res 22 conformer A is PRO and conformer B is SER – is mutation justified?

APRO negative density around CG

BSER negative density around OG

BSER C-N distance 1.24 (1.33), N-CA-CB 103 (110)

res 23 CD-OE2-HE2 88.47 bad angle, can be another conformer to fit green density, also there are non-spherical density

res 24 just some green noise on main chain

res 25 different residues A LEU B ILE

BILE peptide plane deviation > 4 sigma

positive density around CG, CD2, negative density around CD1 BIG

res 26 lots of positive and negative density around SG

res 28 negative density around HG1 on other side is positive – rotate H

res 29 TYR on the side chain the rings are not well fitted - there are already 3 altlocs can add a conformer, refit? BIG

BTYR H with 0.4 A from N BIG ATYR HA floating

Hydrogen mess on the phenyl ring

negative density around CD2/A, C

ATYR N-CA-CB 103 (110), BTYR C-CA-CB 119 (110), CTYR CB-CG-CD2 113 (120)

res 30 HG1 point to red density, may have hydrogen bond with res 26 O

res 31 some green density on C-O bond, can be just some noise

res 32 lots of positive and negative density around SG

green density on Oxygen – some HBond??

res 34 negative density around CA and positive density on N on both altlocs

BILE HA, HB floating BIG, CB1 has only very little density

BILE C-CA-CB angle 122 (111), CB-CG1-CD1 124 (113), O-C-N 131, CG2 methyl group geometry not good, CG2-HG23 too long

AILE C-CA-CB 103

res 36 red and green density around ring, can be improve

Green and red densities on CB Hydrogens (CH2 can be rotated to better fit densities)

res 37 BGLY H floating - BIG

AGLY O pointing to negative density and B Oxygen to positive - BIG

res 38 AALA HA floating

BALA CA, O in positive density

res 39 ATHR HA floating BIG

BTHR H, HA floating BIG, O-C-N 115

positive density around C, O on both conformers BIG

negative density on N of conformer A, The OG1 of two conformers can be separated a bit to fit the positive density.

res 40 N-O stick out the peptide plane

res 41 proline – different puckering – red, green – or just better fit

res 42 oxygen a bit longer C=O bond (red green density)

O-C-N(BASP) 132

res 43 AASP CA-CB-CG-OD1 162, HD2 too close to CG

BASP CA-CB-CG-OD1 168 (0), N-O stick out the peptide plane, HA, HD2 floating

res 44 Hydrogen of the ring are not in a plane

res 46 some green density on side of N maybe rotate Hydrogen and make N-H-O HBond to the terminal O, can be two conformers or just re-fit

res 2001 EOH no map fit, also clash with res 46, geometry itself is wrong, C1-C2 2.22, C1-0 1.54

res 2002 EOH no map fit, also clash with res 8 and 11

bad geometry, for altloc A, The distances C1-C2 and C1-O are too long, and the angle O-C1-C2 is too weird, same for altloc B

res 2003 EOH can be improved

res 2004 EOH geometry is wrong, C1-C2 too long

Questionable waters

3112 clash with res 25 BLEU HD12

3006 3016 3017B 3021 3028 3033B 3035 3047 3051 3052B 3054 3071 3072 3083 3085

3088 3092 3093 3095 3096 3098 3101 3109 3110 3111 3112 3113 3114 3115 3116 3117

3118 3119 3120 3121 3123

Water can be improved:

3023 3025 3027 3031 3066B 3076 3081 3082B 3084 3099