!!index array str

"dem"

!entry.dem.unit.atoms table str name str type int typex int resx int flags int seq int elmnt dbl chg

"C" "CZ" 0 1 131072 1 6 0.865500

"OXT" "O2" 0 1 131072 2 8 -0.411300

"O" "O2" 0 1 131072 3 8 -0.411300

"CA" "Ca" 0 1 131072 4 6 1.194000

"H03" "H?" 0 1 131072 5 1 -0.692600

"N" "N2" 0 1 131072 6 7 -1.239700

"H02" "H" 0 1 131072 7 1 0.289100

"H17" "H" 0 1 131072 8 1 0.289100

"CB" "CM" 0 1 131072 9 6 -0.300400

"H04" "HA" 0 1 131072 10 1 0.158800

"H18" "HA" 0 1 131072 11 1 0.158800

"CG" "CM" 0 1 131072 12 6 -0.300400

"H05" "HA" 0 1 131072 13 1 0.158800

"H19" "HA" 0 1 131072 14 1 0.158800

"SD" "S" 0 1 131072 15 16 -0.488200

"CE" "Ce" 0 1 131072 16 6 1.730900

"H06" "H?" 0 1 131072 17 1 -0.421900

"H20" "H?" 0 1 131072 18 1 -0.421900

"H22" "H?" 0 1 131072 19 1 -0.421900

"C5'" "CT" 0 1 131072 20 6 -0.493400

"H07" "H1" 0 1 131072 21 1 0.190300

"H21" "H1" 0 1 131072 22 1 0.190300

"C4'" "CT" 0 1 131072 23 6 0.036100

"H08" "H1" 0 1 131072 24 1 0.204600

"O4'" "OS" 0 1 131072 25 8 -0.254200

"C3'" "CT" 0 1 131072 26 6 0.212600

"H09" "H1" 0 1 131072 27 1 0.058600

"O3'" "OH" 0 1 131072 28 8 -0.625200

"H10" "HO" 0 1 131072 29 1 0.385700

"C2'" "CT" 0 1 131072 30 6 0.262500

"H11" "H1" 0 1 131072 31 1 0.075000

"O2'" "OH" 0 1 131072 32 8 -0.687800

"H12" "HO" 0 1 131072 33 1 0.462700

"C1'" "CT" 0 1 131072 34 6 -0.060600

"H13" "H2" 0 1 131072 35 1 0.152000

"N1" "NC" 0 1 131072 36 7 -0.666700

"C2" "CQ" 0 1 131072 37 6 0.567600

"H14" "H5" 0 1 131072 38 1 0.009700

"N3" "NC" 0 1 131072 39 7 -0.592100

"C4" "CB" 0 1 131072 40 6 0.189500

"C5" "CB" 0 1 131072 41 6 0.191000

"C6" "CA" 0 1 131072 42 6 0.584300

"N6" "N2" 0 1 131072 43 7 -0.851600

"H15" "H" 0 1 131072 44 1 0.406500

"H16" "H" 0 1 131072 45 1 0.406500

"N7" "NB" 0 1 131072 46 7 -0.602600

"C8" "CK" 0 1 131072 47 6 0.152900

"H01" "H5" 0 1 131072 48 1 0.191600

"N9" "N\*" 0 1 131072 49 7 0.010000

!entry.dem.unit.atomspertinfo table str pname str ptype int ptypex int pelmnt dbl pchg

"C" "CZ" 0 -1 0.0

"OXT" "O2" 0 -1 0.0

"O" "O2" 0 -1 0.0

"CA" "Ca" 0 -1 0.0

"H03" "H?" 0 -1 0.0

"N" "N2" 0 -1 0.0

"H02" "H" 0 -1 0.0

"H17" "H" 0 -1 0.0

"CB" "CM" 0 -1 0.0

"H04" "HA" 0 -1 0.0

"H18" "HA" 0 -1 0.0

"CG" "CM" 0 -1 0.0

"H05" "HA" 0 -1 0.0

"H19" "HA" 0 -1 0.0

"SD" "S" 0 -1 0.0

"CE" "Ce" 0 -1 0.0

"H06" "H?" 0 -1 0.0

"H20" "H?" 0 -1 0.0

"H22" "H?" 0 -1 0.0

"C5'" "CT" 0 -1 0.0

"H07" "H1" 0 -1 0.0

"H21" "H1" 0 -1 0.0

"C4'" "CT" 0 -1 0.0

"H08" "H1" 0 -1 0.0

"O4'" "OS" 0 -1 0.0

"C3'" "CT" 0 -1 0.0

"H09" "H1" 0 -1 0.0

"O3'" "OH" 0 -1 0.0

"H10" "HO" 0 -1 0.0

"C2'" "CT" 0 -1 0.0

"H11" "H1" 0 -1 0.0

"O2'" "OH" 0 -1 0.0

"H12" "HO" 0 -1 0.0

"C1'" "CT" 0 -1 0.0

"H13" "H2" 0 -1 0.0

"N1" "NC" 0 -1 0.0

"C2" "CQ" 0 -1 0.0

"H14" "H5" 0 -1 0.0

"N3" "NC" 0 -1 0.0

"C4" "CB" 0 -1 0.0

"C5" "CB" 0 -1 0.0

"C6" "CA" 0 -1 0.0

"N6" "N2" 0 -1 0.0

"H15" "H" 0 -1 0.0

"H16" "H" 0 -1 0.0

"N7" "NB" 0 -1 0.0

"C8" "CK" 0 -1 0.0

"H01" "H5" 0 -1 0.0

"N9" "N\*" 0 -1 0.0

!entry.dem.unit.boundbox array dbl

-1.000000

0.0

0.0

0.0

0.0

!entry.dem.unit.childsequence single int

2

!entry.dem.unit.connect array int

0

0

!entry.dem.unit.connectivity table int atom1x int atom2x int flags

1 2 1

1 3 1

4 6 1

6 7 1

6 8 1

9 10 1

9 11 1

9 12 1

12 13 1

12 14 1

15 16 1

15 20 1

16 17 1

16 18 1

16 19 1

20 21 1

20 22 1

20 23 1

23 24 1

23 25 1

23 26 1

25 34 1

26 27 1

26 28 1

26 30 1

28 29 1

30 31 1

30 32 1

30 34 1

32 33 1

34 35 1

34 49 1

36 37 1

36 42 1

37 38 1

37 39 1

39 40 1

40 41 1

40 49 1

41 42 1

41 46 1

42 43 1

43 44 1

43 45 1

46 47 1

47 48 1

47 49 1

!entry.dem.unit.hierarchy table str abovetype int abovex str belowtype int belowx

"U" 0 "R" 1

"R" 1 "A" 1

"R" 1 "A" 2

"R" 1 "A" 3

"R" 1 "A" 4

"R" 1 "A" 5

"R" 1 "A" 6

"R" 1 "A" 7

"R" 1 "A" 8

"R" 1 "A" 9

"R" 1 "A" 10

"R" 1 "A" 11

"R" 1 "A" 12

"R" 1 "A" 13

"R" 1 "A" 14

"R" 1 "A" 15

"R" 1 "A" 16

"R" 1 "A" 17

"R" 1 "A" 18

"R" 1 "A" 19

"R" 1 "A" 20

"R" 1 "A" 21

"R" 1 "A" 22

"R" 1 "A" 23

"R" 1 "A" 24

"R" 1 "A" 25

"R" 1 "A" 26

"R" 1 "A" 27

"R" 1 "A" 28

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"R" 1 "A" 36

"R" 1 "A" 37

"R" 1 "A" 38

"R" 1 "A" 39

"R" 1 "A" 40

"R" 1 "A" 41

"R" 1 "A" 42

"R" 1 "A" 43

"R" 1 "A" 44

"R" 1 "A" 45

"R" 1 "A" 46

"R" 1 "A" 47

"R" 1 "A" 48

"R" 1 "A" 49

!entry.dem.unit.name single str

"SAM"

!entry.dem.unit.positions table dbl x dbl y dbl z

4.489186 -3.028822 1.820186

4.466710 -3.498838 2.853977

4.574601 -2.554874 0.772755

2.450991 -1.745257 -0.684070

1.760521 -2.524723 1.321551

3.416280 -2.097905 -2.738075

3.356114 -1.498424 -3.544903

3.963954 -2.879447 -3.057028

0.283989 -4.275176 -1.655284

-0.496758 -4.605541 -0.993342

1.249872 -4.732033 -1.520874

0.072750 -3.383338 -2.609413

-0.902919 -2.954722 -2.765243

0.871052 -3.066038 -3.256327

-3.409165 -1.258809 -0.618721

-5.247594 0.584093 -0.302391

-7.070328 -0.158549 -0.076183

-5.149213 1.761408 -1.896264

-4.672083 1.661941 1.269227

-1.860244 -0.267062 -0.598575

-2.053205 0.769464 -0.337224

-1.453738 -0.270578 -1.599316

-0.821085 -0.866622 0.345505

-0.703210 -1.916795 0.131856

0.434613 -0.214234 0.078158

-1.058715 -0.645932 1.837727

-2.108888 -0.604192 2.085081

-0.478025 -1.621578 2.643665

0.294878 -2.029059 2.226395

-0.358910 0.694655 2.078994

-0.968876 1.508841 1.706829

-0.060359 0.951657 3.403180

0.066885 0.112122 3.836948

0.877697 0.520829 1.202665

1.608105 -0.072873 1.734089

4.656682 2.333074 -1.624855

4.215230 1.106184 -1.427962

4.719730 0.319042 -1.955424

3.201506 0.722878 -0.663222

2.596057 1.754528 -0.072197

2.947777 3.073913 -0.188890

4.046516 3.349236 -1.015008

4.502912 4.585959 -1.216592

5.290636 4.723633 -1.807171

4.076079 5.363743 -0.768979

2.112516 3.867416 0.572417

1.295190 3.044784 1.112111

0.517705 3.311833 1.795588

1.515534 1.729940 0.755655

!entry.dem.unit.residueconnect table int c1x int c2x int c3x int c4x int c5x int c6x

0 0 0 0 0 0

!entry.dem.unit.residues table str name int seq int childseq int startatomx str restype int imagingx

"SAM" 1 50 1 "?" 0

!entry.dem.unit.residuesPdbSequenceNumber array int

0

!entry.dem.unit.solventcap array dbl

-1.000000

0.0

0.0

0.0

0.0

!entry.dem.unit.velocities table dbl x dbl y dbl z

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

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