Electronic Supplementary Material (ESI) for Metallomics

Supporting Information

Identifying Proteins That Can Form Tyrosine-Cysteine Crosslinks

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A. Computational Details and Results

All structure files in the Protein Data Bank (rcsb.org or ftp.wwpdb.org) were downloaded using a combination of Unix script files and *awk* commands or programs on a MacBook Pro. Two lists of PDB directories were downloaded; a list of all structure files (including directories) and a list of experimental methods (pdb_entry_type.txt). Lists of pdb ids that contained structures of proteins (prot or prot-nuc) determined by diffraction were generated. Eighteen lists were used sequentially for automated sftp downloads (*awk* script piped to command shell) of protein diffraction coordinates.

For a given collection of PDB structure files, *Procheck*[1] was run on each structure and the non-bonded contact file was saved. Each Protein Data Bank file was filtered for resolution and chain(s) designations for input to *Procheck*. At the end of each *Procheck* command, the non-bonded contacts file (*.nb) was copied to a neighboring directory and the rest of the *Procheck* output files were discarded. Once all eighteen lists of PDB file downloads and *Procheck* commands executed the directory of non-bonded contacts was backed up and the PDB and additional *Procheck* files were discarded. As of the date of retrieval and analysis (March 2010) the non-bonded contact directory was 22.3 GB.

Files in the non-bonded contact directory were examined with a series of *awk* scripts that were tailored for specific applications. A final list of PDB files contained in the non-bonded contacts directory was generated and ran each of the *awk* scripts. Each application is discussed below with the output organized in the appropriate appendix.

A1. Tyr-Cys Non-Bonded Contact Search.

For the tyrosine $C_{3,5}$-cysteine S contact, the *awk* filter examined each line of each non-bonded contact file to contain both TYR in field 2 or 5, CE in field 3 or 6, CYS in field 2 or 5, and SG in field 3 or 6; where CE refers to $C_{\varepsilon 1,2}$ and SG refers to S_{γ}. When a line that satisfied these criteria was identified it was printed along with the PDB ID to a single file during the search of all non-bonded contact files. The master file of Tyr-Cys non-bonded contacts was sorted by con-

tact distance. Structures that were reported from an ensemble refinement study[2] were removed from this list due to multiple short contacts generated from backbone conformational sampling. Appendix I contains the raw output from these searches.

A2. Tyr-OH Hydrogen Bond Search.

Hydrogen bonded contacts between tyrosine O_4 and a proton accepting atom of an amino acid side chain were found in the non-bonded contacts files. Two methods were used for filtering; raw filtering of all non-bonded contact files or filtering non-bonded contact files that contain a Tyr-Cys non-bonded contact identified in section A1.

All non-bonded contact files: Two *awk* filters were used to examine each line of each non-bonded contact file. One filter looked for lines that contained both TYR in field 2/5, OH in field 3/6, and either ASP in field 2/5 and OD in field 3/6 or GLU in filed 2/5 and OE in field 3/6; where OH refers to O_η, OD refers to $O_{\delta 1/2}$, and OE refers to $O_{\varepsilon 1,2}$. The output file was collected, sorted, and filtered as two files (Asp/Glu and His hydrogen bonds) with the Tyr-Cys non-bonded contact file and are presented in Appendix II for the hydrogen bonds to histidine residues.

From these files, numerous short Tyr-OH contacts with general bases were identified. Contacts with $N_1(N_{\delta 1})$ and $N_3(N_{\varepsilon 2})$ were more limited, but produced a reasonable list of structures such as DsRed fluorescent protein (1ZGO), cytochrome *bc*1 complex (1ZGY), and carbonic anhydrase II (1TG3) with 2.0-2.2 Å contacts. As reported in the text, contacts were observed for the oxygen-evolving complex of photosystem II (1S5L) Q protein with contacts of 2.4 Å (Tyr 161 and His 190 $N_{\varepsilon 2}$, chain a) and 2.7 Å (Tyr 161 and His 190 $N_{\varepsilon 2}$, chain A). Other tyrosine histidine hydrogen bonds were identified in 1S5L as well; 3.0 Å for photosystem II CP43 protein (Tyr 302 and His 91 $N_{\delta 1}$, chain C) and photosystem II reaction center D2 protein (Tyr 160 and His 189 $N_{\varepsilon 2}$, chain D), 3.1 Å for photosystem II reaction center D2 protein (Tyr 160 and His 189 $N_{\varepsilon 2}$, chain d).

Alternatively, non-bonded contact files that contain a Tyr-Cys contact were then filtered for TyrOH hydrogen bonds to Asp, Glu, or His residues as above. Annotated lines were collected and saved to a master file as above. The results are shown in Appendix III.

B. Non-bonded Contact Energy Calculations

Calculated energies from atomic non-bonded contacts were based on CHARMM forcefield parameterization of atom types using a Leonard-Jones 12-6 potential function.[3] The parameters (σ, collision diameter; ε, well depth) used for carbon came from the CHARMM CA atom type (ε_C, 3.984800 Å; σ_C, -0.070000 kcal/mol) for Tyr $C_{\varepsilon 1/2}$, Trp $C_{\zeta 2}$, and Trp $C_{\delta 1}$ and parameters for sulfur came from the CHARMM S atom type (ε_S, 4.000000 Å; σ_S, -0.450000 kcal/mol) for Cys S_γ. For tyrosine $C_{3,5}$ ($C_{\varepsilon 1/2}$)-cysteine S (S_γ) energies, the well depth (ε_{CS}) was calculated as the geometric mean ($\varepsilon_{CS} = \sqrt{\varepsilon_C \bullet \varepsilon_S}$, -0.520000 kcal/mol) and the collision diameter (σ_{CS}) was calculated as the arithmetic mean ($\sigma_{CS} = ½[\sigma_C + \sigma_S]$, 3.994200 Å). For the tryptophan $C_{\delta 1}$-tryptophyl quinone $C_{\zeta 2}$ energies, the atom types were the same (ε_{CC}, 3.984800 Å; σ_{CC}, -0.1400000 kcal/mol). The combined collision diameter and well depth parameters were implemented in the following equation based on a Leonard-Jones 12-6 potential for non-bonded contacts:

$$E_{nbc} = \varepsilon_{ij} \bullet [(\sigma_{ij}/r_{ij})^{12} - 2 \bullet [(\sigma_{ij}/r_{ij})^{6}] \quad (1)$$

, where ε_{ij} and σ_{ij} are defined above while r_{ij} is the crystallographic interatomic distance.

Degree of bond formation was estimated using C-S and C-C bond distances along with minima from non-bonded contacts. Literature values for the C-S bond length in Tyr-Cys and C-C bond length in tryptophan-tryptophyl quinone were derived from a survey[4] of Cambridge Crystallographic Structure Database (d_{bond}(C-S), C_{ar}-S(2)-C*, 1.773 Å; d_{bond}(C-C), C_{ar}-C_{ar} in biphenyls, 1.487 Å). Ideal non-bonded contact interatomic distances were derived from the distances with the most attractive energies, given as the arithmetic mean of the collision diameters (σ_{CS}, 3.994200 Å; σ_{CC}, 3.984800 Å). Calculation of the % crosslinked distance was calculated as:

$$\%d_{crosslink} = (r_{ij} - d_{bond}(ij))/(\sigma_{ij} - d_{bond}(ij)) \bullet 100 \quad (2)$$

Using these metrics the distance cutoff filter applied to the Tyr-Cys contact search represented 3.5 kcal/mol repulsion ($-E_{nbc}$, eq. 1) with a $\%d_{crosslink}$ of 64% (eq. 2). The interatomic distances

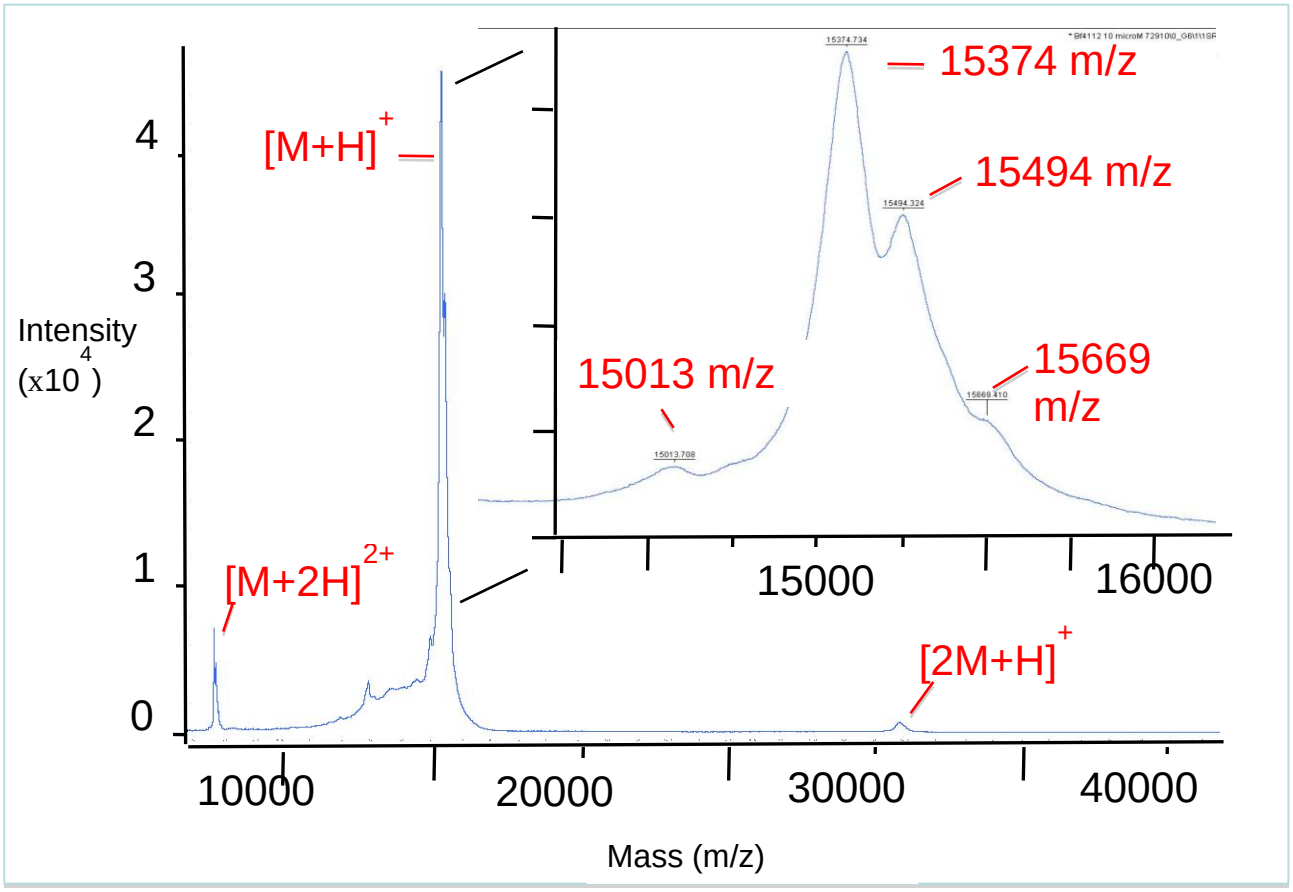
observed in the pre-cofactor structure for galactose oxidase (Tyr-Cys, 1VZ1[5]) gave 0.23 kcal/mol repulsion (78% $d_{crosslink}$) for 3.5 Å and 0.35 kcal/mol attraction (87% $d_{crosslink}$) for 3.7 Å between Tyr 272 $C_{\varepsilon 1}$ and Cys 228 S_{γ}. It should be noted that the crystallographic report shows a structure (not in the PDB) where the Cys 228 S_{γ} seems to be template by Cu^{2+} ion binding, therefore the energetically neutral values for the 3.5 Å and 3.7 Å separations are not surprising. The pre-cofactor structure for methylamine dehydrogenase/MauG cocrystal structure (1L4M[6]), however, showed a repulsion of 12.1 kcal/mol (49% $d_{crosslink}$) for the 2.7 Å separation between Trp 108 $C_{\delta 1}$ and Trq 57 $C_{\zeta 2}$. For the method reported here, non-bonded contact cutoff that provides at least a 3 kcal/mol repulsion seems a reasonable constraint. This cutoff distance is 3.2 Å for Tyr-Cys contacts and 2.9 Å for Trp-Trp contacts.

C. BF4112 Preparation

Once purified, purity of BF4112 was verified by MALDI-MS (predicted mass 15632 Da; MSYYHHHHHHLESTSL (pDEST 17 vector) + YKKAGSEFAL (pCR8 Gateway® vector) + BF4112) shown in Figure S1.

The predicted extinction coefficient of denatured BF4112 was 14440 $M^{-1}cm^{-1}$.[7] We found the absorbance in buffer (20 mM MOPS pH 8.0) to correlate to the absorbance in 6 M guanidine hydrochloride with a ratio of 1.0:1.6, giving an in-buffer extinction coefficient of 8000 $mol^{-1}cm^{-1}$.

Figure S1. MALDI-TOF mass spectrum of recombinantly expressed BF4112.



D. Synthetic and Spectroscopic Details of 3-(S-cysteinyl)-tyrosine

Synthesis of 3-S–Cysteinyltyrosine

The starting materials, L-tyrosine (98%) and L-cystine (99%) were purchased from Sigma. 3-**S**–cysteinyltyrosine was synthesized according to the published literature.[8] In a 250 mL round bottom flask, L-tyrosine (3.62 g, 0.02 mol) and L-cystine (4.81 g, 0.02 mol) were refluxed in 200 mL HBr (Sigma) for 6 hours and the solvent was removed under reduced pressure. The crude product was purified over column chromatography using Dowex 50 W resin and 3 N HCl as the solvent. The product was isolated and compared to the reported UV-vis data. The solvent was removed under reduced pressure and pale white product was obtained in 10% yield. The purity of the product was confirmed by ^{1}H NMR, (300 MHz, D2O, 298 K, TMS): 2.98 (2 H, m), 3.05 (2 H, m), 3.98 (1 H, t), 4.11 (1 H, m), 6.69 (1 H, d), 6.78 (1 H, dd), 7.24 (1 H, d), positive-ion ESI-MS: **m/z** at 301, $\{M+H\}^{+}$

Preparation of 3-S–cysteinyltyrosine Solutions for pH Titrations

The pH range of interest was 3 to 13 unless otherwise indicated. The pH dependence of absorbance was performed with 100 µM 3-S–cysteinyltyrosine solutions in 50 mM phosphate buffer, where the pH was adjusted using HCl and NaOH. The control experiment with parent tyrosine was performed using 100 **µ**M tyrosine in 50 mM phosphate buffer. The pH solutions were analyzed using UV absorbance (1 nm slit width, Hitachi U-3300, fig. S2) and fluorescence emission spectroscopy (1 nm slit widths, 317 nm excitation, Horiba FluoroLog, fig. S3).

Electrochemical characterization of 3-S–cysteinyltyrosine as a function of pH.

Cyclic volatammetry experiments on 100 µM 3-S–cysteinyltyrosine were performed in 50 mM phosphate buffer over a pH range from 2 to 11 with 100 mM KCl. BAS-50 potentiostat/galvanostat was connected to an electrochemical cell containing the 3-S–cysteinyltyrosine solution, freshly polished glassy carbon working electrode, a Ag/AgCl reference electrode, and a Pt counter electrode. The cell was purged with nitrogen before scanning at a rate of 100 mV/s. Experiments yielded one-electron reversible waves (table S1). The pH

dependence of the $E_{1/2}$ was also examined (shown *vs* NHE, Fig. S4). A slope of 30 mV per pH unit was observed suggesting two protons were lost during the reduction. The identity of these protons is unclear, however the $E_{1/2}$ at pH 7.5 is $^{+}$550 mV *vs* NHE. While electrochemical experiments on BF4112 are ongoing, the electrochemistry of 3-S–cysteinyltyrosine suggests Tyr-Cys crosslinks can be active in controlled electron transfer.

Table S1. Potential difference between oxidative and reductive waves (ΔE) relative to pH.

pH	3	4	5	6	7	8	9	10	11
ΔE (mV)	57	56	60	58	54	60	58	57	58

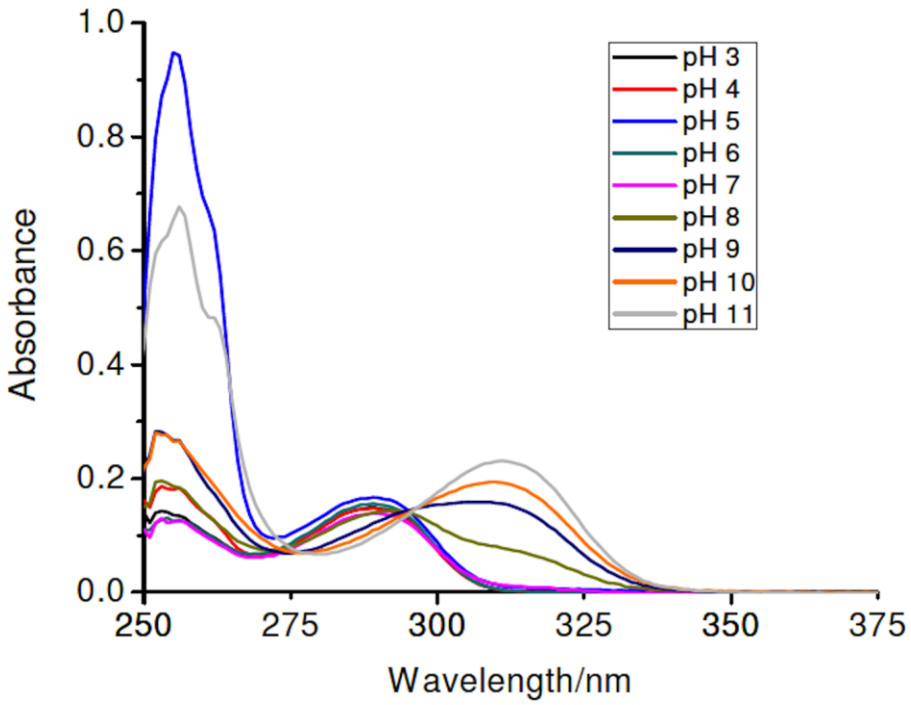


Figure S2. pH dependent absorbance spectrum of 3-(S-cysteinyl)-tyrosine. The orange peak (pH 10, λ_{max} = 317 nm, ε_{317} = 2000 $M^{-1}cm^{-1}$) is similar to the difference peak observed in BF4112.

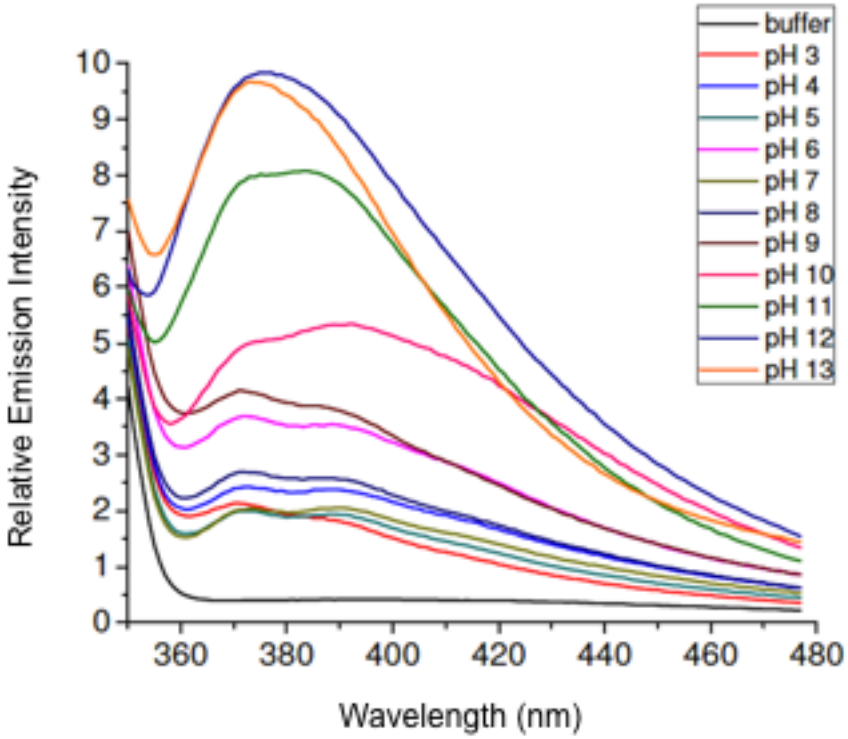


Figure S3. Fluorescence emission spectrum of 3-(S-cystienyl)-tyrosine at various pHs with 317 nm excitation.

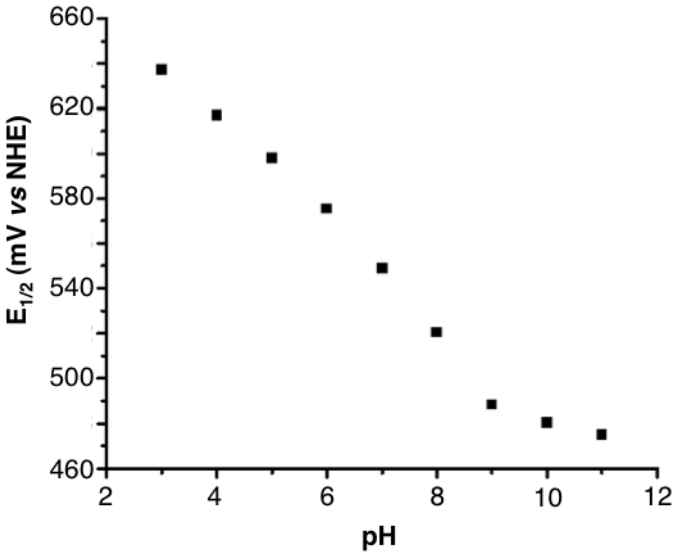


Figure S4. pH dependence of reduction potential of 3-(S-cystienyl)-tyrosine. Reduction potential was estimated as the average between the oxidative and reductive electrochemical wave potentials ($E_{1/2}$) determined at each pH.

E. Proteomic Comparison of Oxygenated and Untreated BF4112 Samples

Both oxygenated and untreated samples of BF4112 were proteolyzed with trypsin at 37°C overnight (Protea Biosystems, BF4112:trypsin = 50:1, 30 ng trypsin in 100 µL, 50 mM ammonium bicarbonate pH 7.9, following Protea protocols). Reaction was quenched with 1 µL 10% trifluoroacetic acid in water and lyophilized. The resulting solid was reconstituted in 50 mM ammonium bicarbonate buffer (pH 7.9), and digested with Glu-C (Protea Biosystems, BF4112:Glu-C = 50:1, 30 ng Glu-C in 100 µL, 50 mM ammonium bicarbonate pH 7.9). Digests (5 µL) were injected onto a C18 capillary column after concentration on a C18 cartridge (Dionex UltiMate 3000). The column was washed with 4.5% acetonitrile for five minutes at 100 nL/min and then developed with a gradient from 4.5% to 45.5% acetonitrile over 30 minutes, where all solvents contained 0.01% trifluoroacetic acid. Eluent from the C18 column (75 µm by 15 cm, 2 µm particle size) was automatically spotted (20 seconds/spot) onto a 96 well MALDI AnchorChip (ProBot, LC Packings/Dionex) mixed with an equal volume of 1% α-cyano-4-hydroxycinnamic acid (50% acetonitrile/0.05% trifluoroacetic acid). Spotted plates were analyzed by MALDI-TOF-MS (Bruker MicroFlex, reflectron mode), where the instrument automatically set initial laser power for 95 sample (+ peptide standards) collection. Samples identified with a mass spectral peak of interest were reshot with optimized mass spectrometer settings for increase mass resolution.

Spectra containing a peak consistent with a crosslinked peptide were compared to analogous retention time spectra of untreated samples and examined for chromatographic resolution. Selected ion chromatograms were generated in IGOR Pro where the average intensities across the peak of interest were tabulated for each samples spectrum (1011.8 ± 2.0 m/z for pepsin digests, 2052.4 ± 2.0 m/z for trypsin/Glu-C digests) and subtracted from similar areas on either side of each peak, for baseline subtraction and eliminating laser power fluctuations. Results for the Trypsin/Glu-C digests are in figure 5 of the main text. Results from the Pepsin digests are in Figure 6.

Both the 1010.7 m/z and the 2052.4 m/z peaks could be assigned to pepsin or trypsin/Glu-C digested alpha-kerritin peptides (1010.7 m/z: keratin, type II cuticular Hb5 40-48, 1010.52 m/z. 2052.4: keratin, type I cuticular Ha2 294-311, 2052.94 m/z); however the occurrence of both peptides only in the oxygenated BF4112 samples would be highly coincidental. The isotope distribution patterns for the trypsin/Glu-C digensted sample were more consistent with the crosslinked bispeptides rather than the alpha-keratin derived peptides (Figure S5).

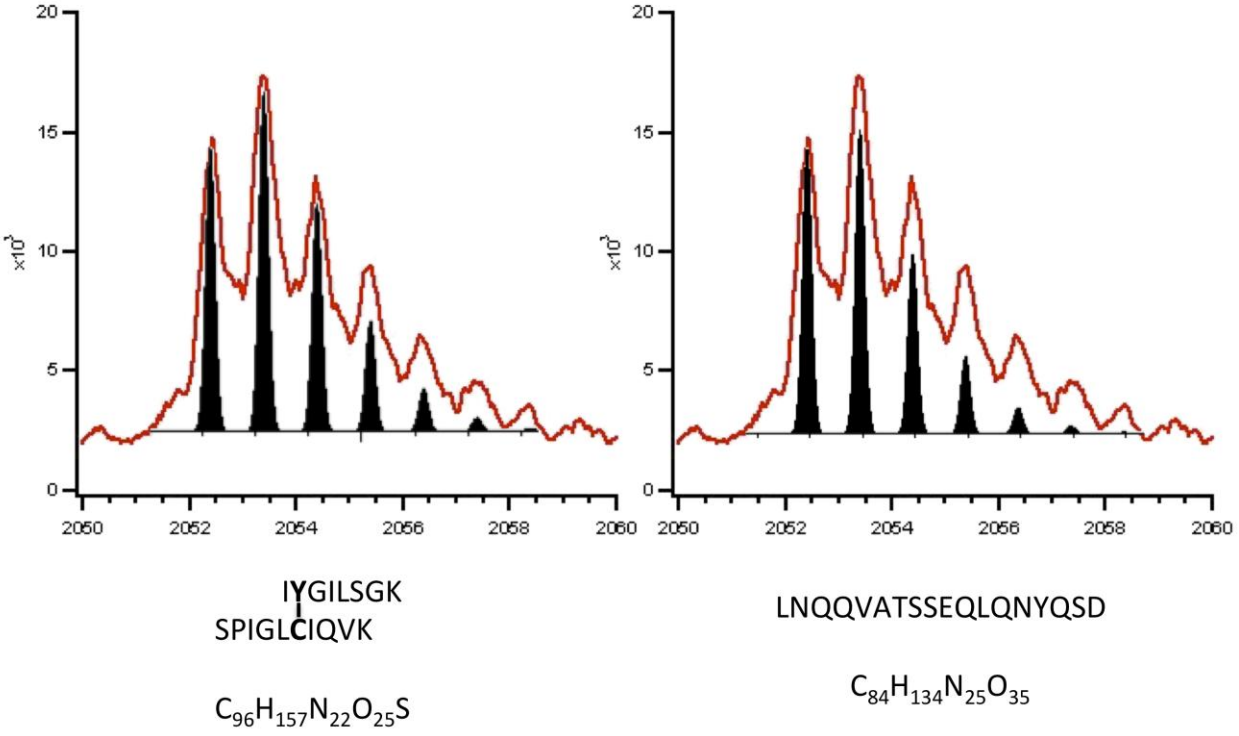


Figure S5. Predicted isotope distribution patterns of crosslinked bispeptide (A) and α-keratin peptide (B) overlaid by the MALDI mass spectrum detected in oxygenated BF4112.

F. References

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G. Appendix I. Tyr-Cys non-bonded contacts

Below is the unedited output from the non-bonded contact search between Tyr $C_{\varepsilon 1/2}$ and Cys S_{γ} with the name of the non-bonded contact file as the first field to designate the PDB accession code for the identified structure. The structure of the output is the non-bonded contact file, residue 1 chain, residue 1, residue 1 atom, residue 2 chain, residue 2, residue 2 atom, interatomic distance, followed by 4 columns of *Procheck* specific output. The list is sorted in ascending interatomic distances.

1zj8.nb	A	/A0069-TYR CE2	A	/A0161-CYS SG	1.6	SS	92	7.6	270
1zj8.nb	B	/B0069-TYR CE1	B	/B0161-CYS SG	1.6	SS	92	7.8	2636
3f29.nb	A	/A0303-TYR CE2	A	/A0305-CYS SG	1.6	SS	2	6.3	2264
3f29.nb	B	/B0303-TYR CE2	B	/B0305-CYS SG	1.6	SS	2	6.3	5792
1goh.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.7	SS	44	5.2	1247
2eib.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.7	SS	44	5.3	1248
2jkx.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.7	SS	44	5.3	1531
2ot4.nb	A	/A0303-TYR CE2	A	/A0305-CYS SG	1.7	SS	2	6.3	1269
2ot4.nb	B	/B0303-TYR CE2	B	/B0305-CYS SG	1.7	SS	2	6.3	3467
2zo5.nb	A	/A0303-TYR CE2	A	/A0305-CYS SG	1.7	SS	2	6.2	1275
2zo5.nb	B	/B0303-TYR CE2	B	/B0305-CYS SG	1.7	SS	2	6.3	3469
3d1i.nb	A	/A0303-TYR CE2	A	/A0305-CYS SG	1.7	SS	2	6.3	1279
3d1i.nb	B	/B0303-TYR CE2	B	/B0305-CYS SG	1.7	SS	2	6.2	3483
3fo3.nb	A	/A0303-TYR CE2	A	/A0305-CYS SG	1.7	SS	2	6.3	1269
3fo3.nb	B	/B0303-TYR CE2	B	/B0305-CYS SG	1.7	SS	2	6.3	3466
3gm6.nb	A	/A0303-TYR CE2	A	/A0305-CYS SG	1.7	SS	2	6.4	1242
3gm6.nb	B	/B0303-TYR CE2	B	/B0305-CYS SG	1.7	SS	2	6.4	3382
1gof.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.8	SS	44	5.3	1262
1gog.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.8	SS	44	5.3	1240
1t2x.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.8	SS	44	5.3	1212
1zj9.nb	A	/A0069-TYR CE1	A	/A0161-CYS SG	1.8	SS	92	7.9	276
2eic.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.8	SS	44	5.1	1141
2eid.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.8	SS	44	5.3	1400
2eie.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	1.8	SS	44	5.3	1508
2gh2.nb	A	/A0093-CYS SG	A	/A0157-TYR CE1	1.8	SS	64	4.6	820
2ic1.nb	A	/A0093-CYS SG	A	/A0157-TYR CE1	1.8	SS	64	4.8	575
1zj9.nb	B	/B0069-TYR CE2	B	/B0161-CYS SG	1.9	SS	92	7.7	2722
3eln.nb	A	/A0093-CYS SG	A	/A0157-TYR CE1	1.9	SS	64	4.7	841
2b5h.nb	A	/A0093-CYS SG	A	/A0157-TYR CE1	2.0	SS	64	4.7	819
2vz3.nb	A	/A0228-CYS SG	A	/A0272-TYR CE1	2.1	SS	44	5.3	1311
2atf.nb	A	/A0093-CYS SG	A	/A0157-TYR CE1	2.2	SS	-1	4.6	716
3a59.nb	B	/B0093-CYS SG	B	/B0145-TYR CE1	2.2	SS	52	6.6	1004
2qls.nb	D	/D0093-CYS SG	D	/D0145-TYR CE2	2.3	SS	52	7.2	2199
3h8k.nb	A	/A0083-TYR CE2	A	/A0089-CYS SG	2.3	SS	6	7.3	527
3dww.nb	C	/C0058-TYR CE2	C	/C0059-CYS SG	2.4	SS	1	3.9	1290
1o95.nb	B	/B0126-TYR CE1	B	/B0136-CYS SG	2.5	SS	10	5.7	3652
1rfq.nb	A	/A0169-TYR CE2	A	/A0374-CYS SG	2.5	SS	205	5.2	718
3k8b.nb	B	/B0093-CYS SG	B	/B0145-TYR CE2	2.5	SS	52	6.1	1205
3gck.nb	A	/A0167-CYS SG	A	/A0172-TYR CE2	2.6	SS	5	8.1	891
3ghg.nb	I	/I0008-CYS SG	I	/I0018-TYR CE2	2.6	SS	10	8.9	9280
1fsx.nb	D	/D0693-CYS SG	D	/D0745-TYR CE2	2.7	SS	52	6.6	2572
1hco.nb	B	/B0093-CYS SG	B	/B0145-TYR CE2	2.7	SS	52	7.1	973
1n10.nb	B	/B2027-TYR CE2	B	/B2058-CYS SG	2.7	SS	-1	9.2	928
1qbq.nb	B	/B0338-TYR CE2	B	/B0343-CYS SG	2.7	SS	5	6.9	3481
1spi.nb	A	/A0191-CYS SG	A	/A0193-TYR CE1	2.7	SS	2	6.3	562
3a59.nb	D	/D0093-CYS SG	D	/D0145-TYR CE2	2.7	SS	52	6.7	2206

3lrc.nb	C	/C0093-TYR	CE1	C	/C0097-CYS	SG	2.7	SS	4	6.0	3869
1n9a.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	2.8	SS	5	6.8	2813
2ped.nb	B	/B0167-CYS	SG	B	/B0206-TYR	CE2	2.8	SS	39	8.7	2763
2vwb.nb	B	/B0107-CYS	SG	B	/B0127-TYR	CE2	2.8	SS	20	7.7	2591
3chk.nb	A	/A0245-CYS	SG	A	/A0282-TYR	CE1	2.8	SS	37	5.8	1770
3fs4.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	2.8	SS	52	6.2	1350
3lrc.nb	A	/A0093-TYR	CE1	A	/A0097-CYS	SG	2.8	SS	4	6.0	480
3lrc.nb	B	/B0093-TYR	CE1	B	/B0097-CYS	SG	2.8	SS	4	6.0	2174
3lrc.nb	D	/D0093-TYR	CE1	D	/D0097-CYS	SG	2.8	SS	4	6.0	5559
1a4f.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	2.9	SS	52	6.1	1220
1ab8.nb	B	/B1058-CYS	SG	B	/B1073-TYR	CE1	2.9	SS	-1	4.5	1686
1amo.nb	A	/A0105-TYR	CE1	A	/A0228-CYS	SG	2.9	SS	123	8.0	257
1amo.nb	B	/B0105-TYR	CE1	B	/B0228-CYS	SG	2.9	SS	123	8.0	3038
1bhy.nb	A	/A0436-TYR	CE2	A	/A0462-CYS	SG	2.9	SS	26	8.7	1365
1clp.nb	A	/A0120-TYR	CE2	A	/A0125-CYS	SG	2.9	SS	5	8.4	468
1fhj.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	2.9	SS	52	7.1	2567
1ft1.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	2.9	SS	5	6.8	3809
1ft2.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	2.9	SS	5	6.7	2845
1g08.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	2.9	SS	52	7.1	1136
1g08.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	2.9	SS	52	7.0	2493
1hho.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	2.9	SS	52	6.1	1173
1iyj.nb	B	/B2747-CYS	SG	B	/B2937-TYR	CE1	2.9	SS	-1	4.6	1367
1iyj.nb	D	/D2747-CYS	SG	D	/D2937-TYR	CE1	2.9	SS	-1	4.6	3657
1kya.nb	B	/B0116-TYR	CE1	B	/B0205-CYS	SG	2.9	SS	89	7.6	2619
1mko.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	2.9	SS	52	6.2	3034
1n95.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	2.9	SS	5	6.8	2819
1o1r.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	2.9	SS	5	6.8	4385
1o1s.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	2.9	SS	5	6.7	4400
1o5m.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	2.9	SS	5	6.8	4409
1ojt.nb	A	/A0436-TYR	CE2	A	/A0462-CYS	SG	2.9	SS	26	8.7	1573
1spi.nb	C	/C0191-CYS	SG	C	/C0193-TYR	CE1	2.9	SS	2	6.5	2890
1tbg.nb	A	/A0114-CYS	SG	A	/A0124-TYR	CE1	2.9	SS	10	8.6	491
1ui7.nb	B	/B0323-TYR	CE1	B	/B0343-CYS	SG	2.9	SS	20	4.9	4635
2f8x.nb	C	/C0058-CYS	SG	C	/C0060-TYR	CE1	2.9	SS	2	6.4	235
2hgu.nb	T	/T0069-CYS	SG	T	/T0076-TYR	CE1	2.9	SS	7	7.8	8862
2ic3.nb	A	/A0038-CYS	SG	A	/A0144-TYR	CE2	2.9	SS	106	8.2	142
2icr.nb	D	/D0119-CYS	SG	D	/D0121-TYR	CE1	2.9	SS	2	6.7	4507
2ped.nb	A	/A0167-CYS	SG	A	/A0206-TYR	CE1	2.9	SS	39	8.8	953
2vhn.nb	N	/N0100-CYS	SG	N	/N0112-TYR	CE1	2.9	SS	12	7.1	6732
3brg.nb	C	/C0098-CYS	SG	C	/C0100-TYR	CE1	2.9	SS	2	6.5	323
3h0g.nb	B	/B0417-TYR	CE1	B	/B0421-CYS	SG	2.9	SS	4	6.2	6567
3ink.nb	C	/C0105-CYS	SG	C	/C0107-TYR	CE1	2.9	SS	2	6.1	407
3ink.nb	D	/D0105-CYS	SG	D	/D0107-TYR	CE1	2.9	SS	2	5.9	893
1a5c.nb	A	/A0180-TYR	CE1	A	/A0184-CYS	SG	3.0	SS	4	6.4	784
1d2h.nb	D	/D0282-CYS	SG	D	/D0283-TYR	CE1	3.0	SS	1	3.8	4305
1dqu.nb	A	/A0371-TYR	CE2	A	/A0377-CYS	SG	3.0	SS	6	9.4	1522
1ex5.nb	B	/B0173-TYR	CE1	B	/B0177-CYS	SG	3.0	SS	4	6.4	2184
1fhj.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	3.0	SS	52	7.1	1178
1hc1.nb	E	/E0046-TYR	CE1	E	/E0098-CYS	SG	3.0	SS	52	7.6	10399
1hni.nb	B	/B0038-CYS	SG	B	/B0144-TYR	CE2	3.0	SS	106	8.7	2199
1iyj.nb	B	/B2531-TYR	CE1	B	/B2535-CYS	SG	3.0	SS	4	6.6	608
1iyj.nb	D	/D2531-TYR	CE1	D	/D2535-CYS	SG	3.0	SS	4	6.6	2897
1j3k.nb	C	/C0494-CYS	SG	C	/C0525-TYR	CE2	3.0	SS	31	8.8	3918
1jcq.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	3.0	SS	5	6.8	3826
1jpi.nb	A	/A0308-CYS	SG	A	/A0342-TYR	CE2	3.0	SS	34	7.8	1951
1ksg.nb	B	/B0081-TYR	CE1	B	/B0086-CYS	SG	3.0	SS	5	6.7	1231

1kya.nb	C	/C0116-TYR	CE1	C	/C0205-CYS	SG	3.0	SS	89	7.6	4641
1kya.nb	D	/D0116-TYR	CE1	D	/D0205-CYS	SG	3.0	SS	89	7.6	6675
1mko.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	3.0	SS	52	6.3	1439
1nl4.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	3.0	SS	5	7.0	2767
1ns6.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	3.0	SS	52	6.3	1231
1nxk.nb	A	/A0258-CYS	SG	A	/A0260-TYR	CE1	3.0	SS	2	5.8	879
1o1t.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	3.0	SS	5	6.8	4248
1si4.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	3.0	SS	52	7.1	1522
1spi.nb	B	/B0191-CYS	SG	B	/B0193-TYR	CE1	3.0	SS	2	6.5	1723
1xdl.nb	A	/A0173-TYR	CE1	A	/A0177-CYS	SG	3.0	SS	4	7.0	662
1xdl.nb	Z	/Z0173-TYR	CE1	Z	/Z0177-CYS	SG	3.0	SS	4	7.0	9788
1y8i.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.0	SS	52	6.9	2669
1yvq.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.0	SS	52	7.2	3466
2a5a.nb	A	/A0044-CYS	SG	A	/A0054-TYR	CE1	3.0	SS	10	8.0	291
2bed.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	3.0	SS	5	6.7	3636
2d2d.nb	B	/B0044-CYS	SG	B	/B0054-TYR	CE2	3.0	SS	10	7.8	1740
2fix.nb	L	/L0116-CYS	SG	L	/L0139-TYR	CE1	3.0	SS	23	7.7	4035
2gt7.nb	B	/B0044-CYS	SG	B	/B0054-TYR	CE1	3.0	SS	10	8.2	2221
2r7z.nb	G	/G0038-CYS	SG	G	/G0044-TYR	CE1	3.0	SS	6	4.8	12393
2ri4.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.0	SS	52	6.9	2246
2vhm.nb	N	/N0100-CYS	SG	N	/N0112-TYR	CE1	3.0	SS	12	7.1	6712
2vwb.nb	A	/A0107-CYS	SG	A	/A0127-TYR	CE2	3.0	SS	20	7.6	432
2z9l.nb	B	/B0044-CYS	SG	B	/B0054-TYR	CE1	3.0	SS	10	7.5	1937
3cew.nb	A	/A0052-TYR	CE2	A	/A0098-CYS	SG	3.0	SS	46	4.8	297
3cew.nb	B	/B0052-TYR	CE2	B	/B0098-CYS	SG	3.0	SS	46	4.8	851
3cew.nb	C	/C0052-TYR	CE2	C	/C0098-CYS	SG	3.0	SS	46	4.8	1418
3cew.nb	D	/D0052-TYR	CE2	D	/D0098-CYS	SG	3.0	SS	46	4.8	1974
3cue.nb	K	/K0061-TYR	CE1	K	/K0065-CYS	SG	3.0	SS	4	6.3	6395
3cue.nb	W	/W0061-TYR	CE1	W	/W0065-CYS	SG	3.0	SS	4	6.3	13862
3d17.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	3.0	SS	52	6.7	1126
3d1a.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.0	SS	52	6.9	2494
3dga.nb	D	/D0494-CYS	SG	D	/D0525-TYR	CE2	3.0	SS	31	9.1	4612
3eok.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	3.0	SS	52	6.5	1176
3eu1.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.0	SS	52	6.5	2219
3eu5.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	3.0	SS	5	7.0	2947
3f8s.nb	A	/A0432-TYR	CE1	A	/A0444-CYS	SG	3.0	SS	12	4.5	1608
3fpx.nb	A	/A0116-TYR	CE1	A	/A0205-CYS	SG	3.0	SS	89	7.3	854
3g5u.nb	B	/B0397-TYR	CE2	B	/B0427-CYS	SG	3.0	SS	30	9.2	6471
3gut.nb	G	/G0036-TYR	CE1	G	/G0120-CYS	SG	3.0	SS	84	5.3	6368
3gxf.nb	C	/C0313-TYR	CE1	C	/C0342-CYS	SG	3.0	SS	29	6.3	5719
3ic0.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.0	SS	52	6.9	3317
3ic2.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.0	SS	52	7.9	2767
1byg.nb	A	/A0223-CYS	SG	A	/A0263-TYR	CE1	3.1	SS	-1	5.1	171
1cx2.nb	D	/D0055-TYR	CE2	D	/D0057-CYS	SG	3.1	SS	2	7.0	7207
1d8e.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	3.1	SS	5	7.0	3039
1epv.nb	A	/A0265-TYR	CE2	A	/A0311-CYS	SG	3.1	SS	46	7.6	1442
1fq3.nb	A	/A0168-CYS	SG	A	/A0175-TYR	CE1	3.1	SS	-1	7.3	593
1g0a.nb	D	/D0093-CYS	SG	D	/D0145-TYR	CE2	3.1	SS	52	7.3	2636
1ikn.nb	A	/A0036-TYR	CE1	A	/A0120-CYS	SG	3.1	SS	84	5.1	113
1ivw.nb	B	/B0323-TYR	CE1	B	/B0343-CYS	SG	3.1	SS	20	5.0	4702
1j3k.nb	D	/D0494-CYS	SG	D	/D0525-TYR	CE2	3.1	SS	31	8.8	5533
1jpe.nb	A	/A0042-TYR	CE2	A	/A0103-CYS	SG	3.1	SS	61	8.1	249
1kig.nb	I	/I0549-TYR	CE2	I	/I0559-CYS	SG	3.1	SS	10	9.4	1265
1kzo.nb	B	/B0338-TYR	CE2	B	/B0343-CYS	SG	3.1	SS	5	7.0	3995
1ld7.nb	B	/B0838-TYR	CE2	B	/B0843-CYS	SG	3.1	SS	5	6.9	4094
1lfq.nb	B	/B0093-CYS	SG	B	/B0145-TYR	CE2	3.1	SS	52	6.6	1059

1ljw.nb	B	/B0093-CYS SG	B	/B0145-TYR CE2	3.1	SS	52	6.6	1549
1nb7.nb	A	/A0004-TYR CE1	A	/A0279-CYS SG	3.1	SS	275	7.3	31
1orr.nb	B	/B0287-CYS SG	B	/B0333-TYR CE2	3.1	SS	46	9.0	2793
1pj0.nb	A	/A0194-TYR CE2	A	/A0268-CYS SG	3.1	SS	74	8.6	1146
1qxd.nb	B	/B0093-CYS SG	B	/B0145-TYR CE2	3.1	SS	52	6.4	1346
1qxd.nb	D	/D0093-CYS SG	D	/D0145-TYR CE2	3.1	SS	52	6.6	2905
1qxe.nb	B	/B0093-CYS SG	B	/B0145-TYR CE2	3.1	SS	52	6.8	1589
1s3s.nb	B	/B0105-CYS SG	B	/B0173-TYR CE2	3.1	SS	6810	3.3	2035
1s63.nb	B	/B0338-TYR CE2	B	/B0343-CYS SG	3.1	SS	5	6.9	4293
1sft.nb	B	/B0265-TYR CE2	B	/B0311-CYS SG	3.1	SS	46	7.7	3293
1tn6.nb	B	/B0838-TYR CE2	B	/B0843-CYS SG	3.1	SS	5	6.9	4338
1ui7.nb	A	/A0323-TYR CE1	A	/A0343-CYS SG	3.1	SS	20	4.9	1726
1uk2.nb	A	/A0044-CYS SG	A	/A0054-TYR CE1	3.1	SS	10	7.9	253
1wcm.nb	G	/G0038-CYS SG	G	/G0044-TYR CE1	3.1	SS	6	5.1	12039
1wmp.nb	A	/A0323-TYR CE1	A	/A0343-CYS SG	3.1	SS	20	5.0	1685
1wmp.nb	B	/B0323-TYR CE1	B	/B0343-CYS SG	3.1	SS	20	4.9	4603
1xdl.nb	C	/C0173-TYR CE1	C	/C0177-CYS SG	3.1	SS	4	6.6	3281
1xdl.nb	X	/X0173-TYR CE1	X	/X0177-CYS SG	3.1	SS	4	6.6	7212
1y1w.nb	G	/G0038-CYS SG	G	/G0044-TYR CE1	3.1	SS	6	5.0	12117
2aei.nb	L	/L0068-TYR CE1	L	/L0070-CYS SG	3.1	SS	2	6.8	309
2apj.nb	D	/D0255-TYR CE2	D	/D0260-CYS SG	3.1	SS	5	7.2	7770
2b1x.nb	A	/A0061-TYR CE1	A	/A0096-CYS SG	3.1	SS	35	9.7	351
2b24.nb	E	/E0061-TYR CE2	E	/E0096-CYS SG	3.1	SS	35	9.9	5180
2b8k.nb	G	/G0038-CYS SG	G	/G0044-TYR CE1	3.1	SS	6	5.1	12099
2c20.nb	D	/D0213-TYR CE2	D	/D0220-CYS SG	3.1	SS	7	7.1	5046
2c3s.nb	A	/A0044-CYS SG	A	/A0054-TYR CE1	3.1	SS	10	8.3	305
2cvt.nb	A	/A0429-CYS SG	A	/A0741-TYR CE1	3.1	SS	-1	6.5	1583
2d5g.nb	F	/F0760-CYS SG	F	/F0790-TYR CE1	3.1	SS	30	8.6	1399
2dh2.nb	A	/A0321-TYR CE2	A	/A0330-CYS SG	3.1	SS	9	9.1	1127
2e4y.nb	A	/A0099-CYS SG	A	/A0104-TYR CE2	3.1	SS	5	6.8	373
2f0y.nb	B	/B0338-TYR CE2	B	/B0343-CYS SG	3.1	SS	5	6.8	3525
2f8x.nb	C	/C0054-CYS SG	C	/C0188-TYR CE1	3.1	SS	134	9.6	216
2h5u.nb	A	/A0116-TYR CE1	A	/A0205-CYS SG	3.1	SS	-1	7.5	964
2jbp.nb	J	/J0258-CYS SG	J	/J0260-TYR CE1	3.1	SS	2	5.8	10641
2r80.nb	D	/D0093-CYS SG	D	/D0145-TYR CE2	3.1	SS	52	7.1	3505
2r93.nb	G	/G0038-CYS SG	G	/G0044-TYR CE1	3.1	SS	6	4.7	12342
2vcp.nb	A	/A0133-TYR CE1	A	/A0374-CYS SG	3.1	SS	241	7.0	560
2vj1.nb	A	/A0044-CYS SG	A	/A0054-TYR CE1	3.1	SS	10	8.1	289
2w8o.nb	A	/A0106-TYR CE2	A	/A0110-CYS SG	3.1	SS	4	6.6	255
2wob.nb	E	/E0019-CYS SG	E	/E0132-TYR CE1	3.1	SS	113	7.1	1750
2z9j.nb	A	/A0044-CYS SG	A	/A0054-TYR CE1	3.1	SS	10	8.3	328
2zfb.nb	B	/B0093-CYS SG	B	/B0145-TYR CE2	3.1	SS	52	6.9	1011
2zl3.nb	M	/M0079-TYR CE1	M	/M0107-CYS SG	3.1	SS	28	6.9	8653
3b75.nb	D	/D0093-CYS SG	D	/D0145-TYR CE2	3.1	SS	52	7.0	2210
3b75.nb	T	/T0093-CYS SG	T	/T0145-TYR CE2	3.1	SS	52	6.5	5718
3bjw.nb	A	/A0073-TYR CE1	A	/A0096-CYS SG	3.1	SS	22	7.1	386
3bjw.nb	A	/A0120-TYR CE2	A	/A0126-CYS SG	3.1	SS	5	9.1	606
3bjw.nb	C	/C0073-TYR CE1	C	/C0096-CYS SG	3.1	SS	22	6.9	1741
3bjw.nb	F	/F0073-TYR CE1	F	/F0096-CYS SG	3.1	SS	22	7.4	3630
3coj.nb	A	/A1697-CYS SG	A	/A1703-TYR CE1	3.1	SS	6	8.9	1016
3dih.nb	A	/A0064-TYR CE1	A	/A0086-CYS SG	3.1	SS	22	7.2	433
3div.nb	A	/A0116-TYR CE1	A	/A0205-CYS SG	3.1	SS	-1	7.5	1023
3dw8.nb	F	/F0020-CYS SG	F	/F0092-TYR CE2	3.1	SS	72	8.7	9459
3e37.nb	B	/B0340-TYR CE2	B	/B0345-CYS SG	3.1	SS	5	6.8	4487
3e73.nb	A	/A0214-TYR CE1	A	/A0264-CYS SG	3.1	SS	50	4.7	1103
3gou.nb	D	/D0093-CYS SG	D	/D0145-TYR CE2	3.1	SS	52	6.8	2315

3gut.nb	C	/C0036-TYR CE1	C	/C0120-CYS SG	3.1	SS	84	5.2	2189
3gxf.nb	B	/B0313-TYR CE2	B	/B0342-CYS SG	3.1	SS	29	7.7	3575
3gxn.nb	A	/A0200-TYR CE2	A	/A0202-CYS SG	3.1	SS	2	6.4	783
3gxn.nb	B	/B0200-TYR CE2	B	/B0202-CYS SG	3.1	SS	2	6.4	2422
3gxt.nb	A	/A0200-TYR CE2	A	/A0202-CYS SG	3.1	SS	2	6.4	800
3iag.nb	C	/C0098-CYS SG	C	/C0100-TYR CE1	3.1	SS	2	6.5	325
3k48.nb	R	/R0009-TYR CE1	R	/R0014-CYS SG	3.1	SS	5	8.2	1461

H. Appendix II. TyrOH hydrogen bonds to His $N_{\delta 1}$ or $N_{\varepsilon 2}$.

Below is the unedited output from the hydrogen bond (non-bonded contact) search between Tyr O_η and His $N_{\delta 1}/N_{\varepsilon 2}$, up to a 2.5 Å interatomic distance, with the name of the non-bonded contact file as the first field to designate the PDB accession code for the identified structure. The structure of the output is the non-bonded contact file, residue 1 chain, residue 1, residue 1 atom, residue 2 chain, residue 2, residue 2 atom, interatomic distance, followed by 4 columns of *Procheck* specific output. The list is sorted in ascending interatomic distances.

1zgo.nb	B	/B0041-HIS ND1	B	/B0214-TYR OH	2.0	SS	-1	7.5	1494
1bgy.nb	C	/C0107-TYR OH	C	/C0308-HIS ND1	2.1	SS	201	9.6	3909
1bgy.nb	O	/O0107-TYR OH	O	/O0308-HIS ND1	2.1	SS	201	9.6	11263
1zgo.nb	A	/A0041-HIS ND1	A	/A0214-TYR OH	2.1	SS	-1	7.5	222
2p1i.nb	A	/A0144-TYR OH	A	/A0213-HIS NE2	2.1	SS	6911.7		425
3e1k.nb	I	/I0118-TYR OH	I	/I0392-HIS ND1	2.1	SS	-1	9.8	6986
1qlu.nb	A	/A0149-HIS ND1	A	/A0408-TYR OH	2.2	SS	25910.1		775
1qlu.nb	B	/B0149-HIS ND1	B	/B0408-TYR OH	2.2	SS	25910.1		3609
1si5.nb	H	/H0602-TYR OH	H	/H0717-HIS ND1	2.2	SS	-1	9.9	521
1tg3.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.2	SS	8611.7		690
1xtc.nb	G	/G0018-TYR OH	G	/G0094-HIS NE2	2.2	SS	7610.4		2209
1ygk.nb	A	/A0079-TYR OH	A	/A0246-HIS ND1	2.2	SS	167	9.0	384
2a77.nb	L	/L0035-HIS ND1	L	/L0037-TYR OH	2.2	SS	2	6.7	226
2i8c.nb	A	/A0017-HIS NE2	A	/A0042-TYR OH	2.2	SS	2510.1		99
2liv.nb	A	/A0076-HIS NE2	A	/A0089-TYR OH	2.2	SS	1311.2		410
3dll.nb	L	/L0037-HIS NE2	L	/L0039-TYR OH	2.2	SS	2	6.6	5581
3e1k.nb	A	/A0118-TYR OH	A	/A0392-HIS ND1	2.2	SS	-1	9.8	468
3e1k.nb	C	/C0118-TYR OH	C	/C0392-HIS ND1	2.2	SS	-1	9.8	2090
3gtl.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.2	SS	2012.4		1532
3hox.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.2	SS	21	8.8	14422
3i3r.nb	B	/B0394-HIS ND1	B	/B0428-TYR OH	2.2	SS	34	9.5	4167
1arh.nb	B	/B0161-TYR OH	B	/B0166-HIS ND1	2.3	SS	5	6.9	2881
1az3.nb	A	/A0072-TYR OH	A	/A0131-HIS ND1	2.3	SS	-110.1		233
1gt8.nb	C	/C0211-TYR OH	C	/C0504-HIS ND1	2.3	SS	293	8.9	9005
1gt8.nb	D	/D0211-TYR OH	D	/D0504-HIS ND1	2.3	SS	293	8.8	12990
1hcy.nb	A	/A0262-TYR OH	A	/A0370-HIS NE2	2.3	SS	10811.5		1274
1hcy.nb	B	/B0262-TYR OH	B	/B0370-HIS NE2	2.3	SS	10811.5		3864
1hcy.nb	C	/C0262-TYR OH	C	/C0370-HIS NE2	2.3	SS	10811.5		6453
1hcy.nb	D	/D0262-TYR OH	D	/D0370-HIS NE2	2.3	SS	10811.5		9043
1hcy.nb	E	/E0262-TYR OH	E	/E0370-HIS NE2	2.3	SS	10811.5		11633
1hcy.nb	F	/F0262-TYR OH	F	/F0370-HIS NE2	2.3	SS	10811.5		14223
1j0b.nb	K	/K0080-HIS ND1	K	/K0317-TYR OH	2.3	SS	237	9.0	13843
1j5w.nb	A	/A0106-HIS ND1	A	/A0167-TYR OH	2.3	SS	6110.6		598
1jc1.nb	C	/C0074-TYR OH	C	/C0199-HIS NE2	2.3	SS	12510.5		2754
1je6.nb	A	/A0260-TYR OH	A	/A0267-HIS ND1	2.3	SS	7	7.4	1022
1l8h.nb	C	/C0107-TYR OH	C	/C0117-HIS ND1	2.3	SS	10	9.4	1766
1l8h.nb	F	/F0107-TYR OH	F	/F0117-HIS ND1	2.3	SS	10	9.3	3757
1lq8.nb	G	/G0089-HIS ND1	G	/G0134-TYR OH	2.3	SS	45	7.8	4285
1nlz.nb	B	/B0142-HIS NE2	B	/B0151-TYR OH	2.3	SS	911.4		1737
1nlz.nb	C	/C0142-HIS NE2	C	/C0151-TYR OH	2.3	SS	911.3		2788
1nlz.nb	D	/D0142-HIS NE2	D	/D0151-TYR OH	2.3	SS	911.4		4040
1nqg.nb	A	/A0172-TYR OH	A	/A0174-HIS ND1	2.3	SS	2	6.7	767
1ntk.nb	C	/C0107-TYR OH	C	/C0308-HIS ND1	2.3	SS	201	9.3	4045
1o6p.nb	B	/B0216-HIS ND1	B	/B0255-TYR OH	2.3	SS	39	8.8	2965
1osg.nb	C	/C0201-TYR OH	C	/C0210-HIS ND1	2.3	SS	9	9.9	1309
1pq6.nb	A	/A0270-HIS NE2	A	/A0335-TYR OH	2.3	SS	6511.7		213

1pqc.nb	D	/D0270-HIS NE2	D	/D0335-TYR OH	2.3	SS	-111.6			3808
1rj7.nb	H	/H0252-HIS ND1	H	/H0304-TYR OH	2.3	SS	52	9.2		3178
1rq5.nb	A	/A0559-TYR OH	A	/A0589-HIS NE2	2.3	SS	3012.8			2363
1tlb.nb	A	/A0201-HIS ND1	A	/A0273-TYR OH	2.3	SS	7210.1			854
1tlv.nb	A	/A0207-HIS ND1	A	/A0265-TYR OH	2.3	SS	-1	9.3		873
1twa.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.3	SS	8	9.8		10096
1twc.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.3	SS	8	9.9		10119
1twg.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.3	SS	810.0			9985
1twh.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.3	SS	8	9.8		9916
1wcm.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.3	SS	21	8.9		13506
1y77.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.3	SS	21	8.9		13559
2acl.nb	B	/B0254-HIS NE2	B	/B0319-TYR OH	2.3	SS	6511.6			1104
2acl.nb	D	/D0254-HIS NE2	D	/D0319-TYR OH	2.3	SS	6511.8			2991
2b63.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.3	SS	21	8.8		13319
2b8k.nb	A	/A0804-TYR OH	A	/A0816-HIS NE2	2.3	SS	1211.3			2921
2b8k.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.3	SS	21	8.9		13569
2c5h.nb	B	/B0211-HIS ND1	B	/B0284-TYR OH	2.3	SS	73	9.6		2185
2cbt.nb	B	/B2045-TYR OH	B	/B2094-HIS NE2	2.3	SS	49	9.6		622
2cjz.nb	A	/A-005-TYR OH	A	/A0312-HIS ND1	2.3	SS	5910.4			16
2dut.nb	A	/A0095-HIS NE2	A	/A0140-TYR OH	2.3	SS	4510.4			339
2dut.nb	B	/B0095-HIS NE2	B	/B0140-TYR OH	2.3	SS	4510.4			1741
2dut.nb	C	/C0095-HIS NE2	C	/C0140-TYR OH	2.3	SS	4510.4			3144
2dut.nb	D	/D0095-HIS NE2	D	/D0140-TYR OH	2.3	SS	4510.4			4547
2f4i.nb	D	/D0079-HIS ND1	D	/D0094-TYR OH	2.3	SS	-1	8.3		3424
2gmx.nb	A	/A0125-HIS ND1	A	/A0320-TYR OH	2.3	SS	195	9.3		493
2i4m.nb	C	/C0174-TYR OH	C	/C0208-HIS ND1	2.3	SS	34	9.9		4403
2i60.nb	G	/G0249-HIS ND1	G	/G0486-TYR OH	2.3	SS	-110.1			380
2ja7.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.3	SS	2012.6			1689
2nzt.nb	A	/A0417-TYR OH	A	/A0428-HIS NE2	2.3	SS	1110.7			1743
2p1i.nb	D	/D0144-TYR OH	D	/D0213-HIS NE2	2.3	SS	6911.7			3673
2r92.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.3	SS	21	8.9		13926
2r93.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.3	SS	2012.8			1698
2rgn.nb	B	/B0217-HIS NE2	B	/B0249-TYR OH	2.3	SS	3212.0			1671
2rve.nb	B	/B0072-TYR OH	B	/B0131-HIS ND1	2.3	SS	5910.6			1153
2v9p.nb	F	/F0482-HIS ND1	F	/F0532-TYR OH	2.3	SS	5010.0			6282
2vit.nb	C	/C0183-HIS ND1	C	/C0195-TYR OH	2.3	SS	1210.1			2190
3bcc.nb	A	/A0154-HIS NE2	A	/A0314-TYR OH	2.3	SS	16012.2			693
3bji.nb	B	/B0247-HIS NE2	B	/B0280-TYR OH	2.3	SS	3311.7			1928
3cd2.nb	A	/A0093-HIS NE2	A	/A0109-TYR OH	2.3	SS	1612.0			507
3csu.nb	A	/A0156-HIS ND1	A	/A0185-TYR OH	2.3	SS	29	7.6		1013
3da4.nb	A	/A0183-HIS NE2	A	/A0188-TYR OH	2.3	SS	510.1			1496
3f8w.nb	A	/A0137-HIS ND1	A	/A0168-TYR OH	2.3	SS	31	8.9		756
3fa3.nb	J	/J0044-TYR OH	J	/J0114-HIS NE2	2.3	SS	7010.7			11265
3fa3.nb	N	/N0044-TYR OH	N	/N0114-HIS NE2	2.3	SS	7010.6			16087
3fcw.nb	E	/E0053-HIS ND1	E	/E0058-TYR OH	2.3	SS	5	8.0		2936
3gbm.nb	B	/B0022-TYR OH	B	/B0111-HIS ND1	2.3	SS	89	8.6		1274
3ggg.nb	C	/C0147-HIS NE2	C	/C5959-TYR OH	2.3	SS	-112.4			4620
3gvy.nb	C	/C0025-TYR OH	C	/C0130-HIS NE2	2.3	SS	10511.9			1553
3hnp.nb	D	/D0018-HIS ND1	D	/D0305-TYR OH	2.3	SS	-1	8.5		4211
3how.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.3	SS	21	9.0		14007
3hxr.nb	A	/A0626-HIS ND1	A	/A0710-TYR OH	2.3	SS	8411.3			2090
3ibj.nb	A	/A0223-TYR OH	A	/A0364-HIS NE2	2.3	SS	14111.8			5
3inb.nb	B	/B0529-TYR OH	B	/B0536-HIS ND1	2.3	SS	7	7.5		2595
3lys.nb	A	/A0108-TYR OH	A	/A0128-HIS ND1	2.3	SS	20	9.3		246
3lys.nb	B	/B0108-TYR OH	B	/B0128-HIS ND1	2.3	SS	20	9.3		682
3lys.nb	C	/C0108-TYR OH	C	/C0128-HIS ND1	2.3	SS	20	9.3		1118

3lys.nb	D	/D0108-TYR OH	D	/D0128-HIS ND1	2.3	SS	20	9.3	1537
3lys.nb	E	/E0108-TYR OH	E	/E0128-HIS ND1	2.3	SS	20	9.3	1978
3lys.nb	F	/F0108-TYR OH	F	/F0128-HIS ND1	2.3	SS	20	9.3	2410
1a8h.nb	A	/A0234-TYR OH	A	/A0265-HIS NE2	2.4	SS	31	11.3	1238
1a8m.nb	C	/C0015-HIS ND1	C	/C0059-TYR OH	2.4	SS	44	8.9	1185
1aqx.nb	B	/B0118-TYR OH	B	/B0162-HIS NE2	2.4	SS	44	10.9	1791
1b4f.nb	A	/A0026-TYR OH	A	/A0059-HIS ND1	2.4	SS	33	10.0	121
1b4f.nb	C	/C0026-TYR OH	C	/C0059-HIS ND1	2.4	SS	-11	0.0	1026
1b4f.nb	D	/D0026-TYR OH	D	/D0059-HIS ND1	2.4	SS	33	9.9	1431
1b6s.nb	B	/B0305-TYR OH	B	/B0317-HIS ND1	2.4	SS	12	8.4	2621
1be3.nb	A	/A0279-HIS ND1	A	/A0284-TYR OH	2.4	SS	5	9.5	1150
1bgy.nb	A	/A0279-HIS ND1	A	/A0284-TYR OH	2.4	SS	5	9.6	1154
1bgy.nb	M	/M0279-HIS ND1	M	/M0284-TYR OH	2.4	SS	5	9.6	8522
1bgy.nb	N	/N0254-HIS ND1	N	/N0325-TYR OH	2.4	SS	71	7.3	10087
1bjm.nb	A	/A0192-HIS ND1	A	/A0195-TYR OH	2.4	SS	3	7.5	966
1cd3.nb	F	/F0077-TYR OH	F	/F0122-HIS ND1	2.4	SS	45	7.1	2704
1ci7.nb	B	/B0174-HIS ND1	B	/B0214-TYR OH	2.4	SS	-1	9.9	2273
1cnb.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.4	SS	71	11.9	292
1cnw.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.4	SS	86	11.6	630
1csj.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.4	SS	15	9.2	520
1cva.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.4	SS	71	11.9	291
1cvb.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.4	SS	71	11.9	284
1cvf.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.4	SS	86	11.7	646
1cx2.nb	B	/B0234-TYR OH	B	/B0309-HIS ND1	2.4	SS	75	10.1	3298
1dbz.nb	C	/C0189-TYR OH	C	/C0278-HIS ND1	2.4	SS	89	9.3	3184
1e1e.nb	A	/A0232-HIS ND1	A	/A0298-TYR OH	2.4	SS	66	9.9	1321
1e2l.nb	A	/A0058-HIS ND1	A	/A0172-TYR OH	2.4	SS	-110	6.0	109
1e4k.nb	C	/C0129-TYR OH	C	/C0131-HIS ND1	2.4	SS	2	6.9	1986
1e5l.nb	B	/B0131-HIS ND1	B	/B0233-TYR OH	2.4	SS	102	8.5	2745
1e5r.nb	A	/A0022-TYR OH	A	/A0071-HIS ND1	2.4	SS	-1	9.0	134
1ein.nb	A	/A0021-TYR OH	A	/A0145-HIS ND1	2.4	SS	124	9.5	149
1eop.nb	A	/A0072-TYR OH	A	/A0131-HIS ND1	2.4	SS	59	10.7	290
1eth.nb	C	/C0271-TYR OH	C	/C0310-HIS ND1	2.4	SS	39	6.1	3428
1f0m.nb	A	/A0026-TYR OH	A	/A0059-HIS ND1	2.4	SS	33	9.9	128
1f5q.nb	B	/B0043-HIS ND1	B	/B0048-TYR OH	2.4	SS	5	8.3	1544
1f9w.nb	A	/A0606-HIS ND1	A	/A0619-TYR OH	2.4	SS	13	7.1	946
1f9w.nb	B	/B0606-HIS ND1	B	/B0619-TYR OH	2.4	SS	13	7.1	2264
1fg9.nb	C	/C0130-HIS ND1	C	/C0155-TYR OH	2.4	SS	-1	9.4	1365
1fg9.nb	D	/D0130-HIS ND1	D	/D0155-TYR OH	2.4	SS	-1	9.2	2071
1fiy.nb	A	/A0402-HIS NE2	A	/A0472-TYR OH	2.4	SS	70	12.1	1899
1frv.nb	C	/C0244-HIS NE2	C	/C0262-TYR OH	2.4	SS	18	9.3	4245
1fv9.nb	A	/A0086-TYR OH	A	/A0093-HIS ND1	2.4	SS	7	7.7	412
1g7k.nb	D	/D0041-HIS ND1	D	/D0214-TYR OH	2.4	SS	-1	7.6	3805
1ggx.nb	C	/C0041-HIS ND1	C	/C0214-TYR OH	2.4	SS	-1	7.6	2788
1gsl.nb	A	/A0073-TYR OH	A	/A0175-HIS ND1	2.4	SS	102	7.0	455
1gt8.nb	B	/B0211-TYR OH	B	/B0504-HIS ND1	2.4	SS	293	8.9	5020
1gyt.nb	A	/A0123-TYR OH	A	/A0176-HIS ND1	2.4	SS	53	9.9	554
1gyt.nb	E	/E0123-TYR OH	E	/E0176-HIS ND1	2.4	SS	53	9.9	9110
1gyt.nb	H	/H0123-TYR OH	H	/H0176-HIS ND1	2.4	SS	53	9.9	15549
1gzu.nb	B	/B0065-HIS ND1	B	/B0247-TYR OH	2.4	SS	-1	9.1	1205
1h4m.nb	X	/X0078-HIS ND1	X	/X0084-TYR OH	2.4	SS	6	9.1	559
1h6v.nb	A	/A0403-HIS ND1	A	/A0422-TYR OH	2.4	SS	19	7.6	1582
1hc1.nb	A	/A0262-TYR OH	A	/A0370-HIS NE2	2.4	SS	108	11.5	1247
1hc1.nb	B	/B0262-TYR OH	B	/B0370-HIS NE2	2.4	SS	108	11.4	3774
1heb.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.4	SS	86	11.7	666
1hg5.nb	A	/A0083-HIS ND1	A	/A0127-TYR OH	2.4	SS	44	9.6	388

1hr6.nb	F	/F0167-HIS	NE2	F	/F0330-TYR	OH	2.4	SS	16312.1		9942
1ii7.nb	A	/A0141-HIS	ND1	A	/A0199-TYR	OH	2.4	SS	58	9.3	832
1iv5.nb	B	/B0227-TYR	OH	B	/B0251-HIS	NE2	2.4	SS	2410.0		441
1j0b.nb	G	/G0080-HIS	ND1	G	/G0317-TYR	OH	2.4	SS	237	9.6	8504
1j0b.nb	G	/G0080-HIS	NE2	G	/G0256-TYR	OH	2.4	SS	17612.3		8502
1j9w.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.4	SS	7111.1		295
1j9w.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.4	SS	8711.6		669
1jc0.nb	C	/C0074-TYR	OH	C	/C0199-HIS	NE2	2.4	SS	12511.0		2589
1jg0.nb	A	/A0147-HIS	ND1	A	/A0181-TYR	OH	2.4	SS	34	9.6	983
1jre.nb	E	/E0107-TYR	OH	E	/E0117-HIS	ND1	2.4	SS	10	9.4	3138
1jts.nb	J	/J0107-TYR	OH	J	/J0117-HIS	ND1	2.4	SS	10	9.5	6514
1jts.nb	M	/M0107-TYR	OH	M	/M0117-HIS	ND1	2.4	SS	10	9.5	8545
1jts.nb	N	/N0107-TYR	OH	N	/N0117-HIS	ND1	2.4	SS	10	9.4	9226
1jts.nb	X	/X0107-TYR	OH	X	/X0117-HIS	ND1	2.4	SS	10	9.4	15994
1jz5.nb	A	/A0357-HIS	ND1	A	/A0392-TYR	OH	2.4	SS	35	8.8	1507
1khv.nb	B	/B0321-HIS	NE2	B	/B0358-TYR	OH	2.4	SS	3711.3		3859
1klj.nb	H	/H0101-HIS	ND1	H	/H0234-TYR	OH	2.4	SS	-1	9.0	731
1kny.nb	A	/A0180-HIS	ND1	A	/A0243-TYR	OH	2.4	SS	63	9.4	852
1kvq.nb	A	/A0177-TYR	OH	A	/A0243-HIS	NE2	2.4	SS	6610.9		1290
1kvs.nb	A	/A0177-TYR	OH	A	/A0243-HIS	NE2	2.4	SS	6610.8		1260
1kyq.nb	C	/C0009-HIS	ND1	C	/C0108-TYR	OH	2.4	SS	-1	9.9	3012
1kzi.nb	B	/B0147-HIS	ND1	B	/B0181-TYR	OH	2.4	SS	34	9.6	2668
1l0l.nb	C	/C0107-TYR	OH	C	/C0308-HIS	ND1	2.4	SS	201	9.4	4069
1l0n.nb	C	/C0107-TYR	OH	C	/C0308-HIS	ND1	2.4	SS	201	9.1	4034
1l8h.nb	A	/A0107-TYR	OH	A	/A0117-HIS	ND1	2.4	SS	10	9.4	430
1l8h.nb	E	/E0107-TYR	OH	E	/E0117-HIS	ND1	2.4	SS	10	9.3	3096
1l8h.nb	G	/G0107-TYR	OH	G	/G0117-HIS	ND1	2.4	SS	10	9.4	4427
1l8h.nb	I	/I0107-TYR	OH	I	/I0117-HIS	ND1	2.4	SS	10	9.4	5758
1l8h.nb	J	/J0107-TYR	OH	J	/J0117-HIS	ND1	2.4	SS	10	9.4	6427
1l8i.nb	H	/H0107-TYR	OH	H	/H0117-HIS	ND1	2.4	SS	10	9.2	5049
1lq8.nb	C	/C0089-HIS	ND1	C	/C0134-TYR	OH	2.4	SS	45	7.7	1652
1m1x.nb	B	/B0115-TYR	OH	B	/B0192-HIS	ND1	2.4	SS	7710.4		3719
1m8v.nb	K	/K0410-HIS	ND1	K	/K0434-TYR	OH	2.4	SS	24	8.1	2736
1mma.nb	A	/A0572-HIS	NE2	A	/A0579-TYR	OH	2.4	SS	711.8		3304
1mql.nb	D	/D0183-HIS	ND1	D	/D0195-TYR	OH	2.4	SS	1210.3		2553
1mqm.nb	G	/G0183-HIS	ND1	G	/G0195-TYR	OH	2.4	SS	1210.3		4345
1mqn.nb	G	/G0183-HIS	ND1	G	/G0195-TYR	OH	2.4	SS	1210.3		4345
1ngs.nb	B	/B0042-HIS	ND1	B	/B0297-TYR	OH	2.4	SS	255	9.7	3112
1nj8.nb	A	/A0053-HIS	NE2	A	/A0250-TYR	OH	2.4	SS	19712.0		253
1nj8.nb	C	/C0053-HIS	NE2	C	/C0250-TYR	OH	2.4	SS	19712.0		3924
1ntk.nb	A	/A0154-HIS	NE2	A	/A0314-TYR	OH	2.4	SS	16011.5		746
1ntm.nb	A	/A0152-TYR	OH	A	/A0243-HIS	ND1	2.4	SS	91	8.8	735
1o95.nb	A	/A0169-TYR	OH	A	/A0172-HIS	ND1	2.4	SS	3	8.9	830
1p9o.nb	B	/B0078-TYR	OH	B	/B0303-HIS	ND1	2.4	SS	-111.4		1837
1peq.nb	A	/A0109-TYR	OH	A	/A0125-HIS	ND1	2.4	SS	16	7.9	471
1peq.nb	A	/A0537-TYR	OH	A	/A0656-HIS	ND1	2.4	SS	119	9.7	2374
1pgz.nb	A	/A0124-TYR	OH	A	/A0168-HIS	ND1	2.4	SS	44	7.8	533
1pq9.nb	A	/A0270-HIS	NE2	A	/A0335-TYR	OH	2.4	SS	6511.2		230
1pq9.nb	D	/D0270-HIS	NE2	D	/D0335-TYR	OH	2.4	SS	-111.5		3822
1pv2.nb	B	/B0049-HIS	ND1	B	/B0281-TYR	OH	2.4	SS	-1	9.8	1106
1qc6.nb	A	/A1071-TYR	OH	A	/A1079-HIS	ND1	2.4	SS	8	7.3	257
1qfc.nb	A	/A0055-TYR	OH	A	/A0223-HIS	NE2	2.4	SS	-111.9		307
1qha.nb	A	/A0417-TYR	OH	A	/A0428-HIS	NE2	2.4	SS	1110.8		1733
1qlt.nb	B	/B0149-HIS	ND1	B	/B0408-TYR	OH	2.4	SS	25910.0		3883
1qol.nb	G	/G0062-TYR	OH	G	/G0138-HIS	ND1	2.4	SS	7610.5		3830
1qqt.nb	A	/A0028-HIS	ND1	A	/A0091-TYR	OH	2.4	SS	63	9.6	188

1rdx.nb	A	/A0164-TYR OH	A	/A0253-HIS ND1	2.4	SS	89	9.7	624
1rfu.nb	B	/B0079-TYR OH	B	/B0246-HIS ND1	2.4	SS	167	9.7	1600
1rj2.nb	G	/G0693-HIS NE2	G	/G0725-TYR OH	2.4	SS	3211.7		3051
1rj5.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.4	SS	6912.7		265
1rj7.nb	I	/I0252-HIS ND1	I	/I0304-TYR OH	2.4	SS	52	9.2	3694
1rj7.nb	J	/J0252-HIS ND1	J	/J0304-TYR OH	2.4	SS	52	9.3	4201
1rm6.nb	E	/E0046-HIS ND1	E	/E0141-TYR OH	2.4	SS	9510.6		8627
1rq5.nb	A	/A0373-TYR OH	A	/A0465-HIS NE2	2.4	SS	9212.4		1057
1rqr.nb	B	/B0211-HIS ND1	B	/B0284-TYR OH	2.4	SS	73	9.7	2217
1rv3.nb	A	/A0347-TYR OH	A	/A0426-HIS ND1	2.4	SS	79	9.2	1574
1rv4.nb	A	/A0347-TYR OH	A	/A0426-HIS ND1	2.4	SS	79	9.1	1579
1rvz.nb	H	/H0522-TYR OH	H	/H0611-HIS ND1	2.4	SS	89	8.7	6694
1s4i.nb	A	/A0088-TYR OH	A	/A0166-HIS NE2	2.4	SS	7811.9		1215
1s5l.nb	a	/a2161-TYR OH	a	/a2190-HIS NE2	2.4	SS	2912.0		9625
1s8e.nb	A	/A0141-HIS ND1	A	/A0199-TYR OH	2.4	SS	58	9.4	851
1sqq.nb	C	/C0107-TYR OH	C	/C0308-HIS ND1	2.4	SS	201	9.3	4118
1sqv.nb	A	/A0154-HIS NE2	A	/A0314-TYR OH	2.4	SS	16011.5		749
1sqx.nb	C	/C0107-TYR OH	C	/C0308-HIS ND1	2.4	SS	201	9.4	4147
1st0.nb	A	/A0217-TYR OH	A	/A0279-HIS ND1	2.4	SS	62	7.0	3051
1sxi.nb	R	/R0223-TYR OH	R	/R0256-HIS ND1	2.4	SS	33	9.7	5132
1t8w.nb	D	/D0209-TYR OH	D	/D0452-HIS ND1	2.4	SS	-1	8.8	6487
1t8w.nb	E	/E0209-TYR OH	E	/E0452-HIS ND1	2.4	SS	-1	8.8	8349
1t8w.nb	F	/F0209-TYR OH	F	/F0452-HIS ND1	2.4	SS	-1	8.8	10207
1t8y.nb	B	/B0209-TYR OH	B	/B0452-HIS ND1	2.4	SS	243	8.8	2732
1t8y.nb	E	/E0209-TYR OH	E	/E0452-HIS ND1	2.4	SS	-1	8.9	8367
1tf2.nb	A	/A0125-HIS ND1	A	/A0364-TYR OH	2.4	SS	23910.2		587
1tls.nb	B	/B0147-HIS ND1	B	/B0181-TYR OH	2.4	SS	34	9.8	2281
1tlw.nb	A	/A0183-TYR OH	A	/A0218-HIS ND1	2.4	SS	35	7.5	624
1tyh.nb	B	/B0050-HIS ND1	B	/B0117-TYR OH	2.4	SS	67	8.6	1409
1u59.nb	A	/A0397-TYR OH	A	/A0611-HIS NE2	2.4	SS	214	9.9	306
1u8c.nb	B	/B1115-TYR OH	B	/B1192-HIS ND1	2.4	SS	7710.3		3814
1uaa.nb	B	/B0334-HIS ND1	B	/B0345-TYR OH	2.4	SS	1110.1		4047
1w2d.nb	A	/A0289-TYR OH	A	/A0305-HIS ND1	2.4	SS	16	8.0	545
1w2f.nb	A	/A0217-TYR OH	A	/A0393-HIS NE2	2.4	SS	17611.4		168
1w8b.nb	L	/L0101-TYR OH	L	/L0115-HIS ND1	2.4	SS	14	7.1	1226
1w8j.nb	B	/B0552-HIS NE2	B	/B0559-TYR OH	2.4	SS	711.8		5356
1y1w.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.4	SS	2012.5		1650
1y1w.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.4	SS	21	8.9	13600
1ygu.nb	B	/B0740-TYR OH	B	/B0827-HIS NE2	2.4	SS	8712.4		2961
1yp4.nb	C	/C0071-TYR OH	C	/C0134-HIS NE2	2.4	SS	-111.5		3847
1z3h.nb	B	/B0513-TYR OH	B	/B0560-HIS NE2	2.4	SS	-112.8		6235
1zc2.nb	A	/A0314-HIS ND1	A	/A0325-TYR OH	2.4	SS	11	7.4	1913
1zdl.nb	A	/A0428-HIS ND1	A	/A0447-TYR OH	2.4	SS	19	7.5	1660
1zxl.nb	A	/A0268-HIS ND1	A	/A0412-TYR OH	2.4	SS	-1	8.6	776
2acl.nb	H	/H0254-HIS NE2	H	/H0319-TYR OH	2.4	SS	6511.5		6774
2ahe.nb	A	/A0196-HIS ND1	A	/A0225-TYR OH	2.4	SS	29	9.8	1154
2ajd.nb	C	/C0735-TYR OH	C	/C0750-HIS ND1	2.4	SS	15	9.4	8686
2ath.nb	B	/B0323-HIS NE2	B	/B0473-TYR OH	2.4	SS	15010.5		1957
2atq.nb	A	/A0138-HIS ND1	A	/A0201-TYR OH	2.4	SS	63	9.1	591
2b2c.nb	B	/B0294-TYR OH	B	/B0299-HIS ND1	2.4	SS	5	6.7	2369
2b3y.nb	A	/A0245-TYR OH	A	/A0267-HIS ND1	2.4	SS	2210.5		1273
2b3y.nb	B	/B0245-TYR OH	B	/B0267-HIS ND1	2.4	SS	2210.5		5163
2bbj.nb	E	/E0115-TYR OH	E	/E0120-HIS ND1	2.4	SS	5	7.8	4288
2bis.nb	A	/A0125-HIS ND1	A	/A0425-TYR OH	2.4	SS	300	8.0	569
2bl7.nb	A	/A0010-HIS ND1	A	/A0035-TYR OH	2.4	SS	25	7.4	49
2bn4.nb	B	/B0289-HIS ND1	B	/B0588-TYR OH	2.4	SS	299	9.5	3669

2brk.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.4	SS	15	9.4		629
2bwe.nb	S	/S0046-TYR OH	S	/S0066-HIS ND1	2.4	SS	20	9.1		3599
2bwe.nb	U	/U0046-TYR OH	U	/U0066-HIS ND1	2.4	SS	20	9.1		4139
2byt.nb	A	/A0535-TYR OH	A	/A0545-HIS NE2	2.4	SS	1012.1			2286
2byt.nb	D	/D0535-TYR OH	D	/D0545-HIS NE2	2.4	SS	1012.1			5865
2c1c.nb	B	/B0184-HIS NE2	B	/B0257-TYR OH	2.4	SS	7810.9			3039
2ckw.nb	A	/A0313-HIS NE2	A	/A0351-TYR OH	2.4	SS	3811.3			1999
2e3k.nb	A	/A0365-HIS ND1	A	/A0368-TYR OH	2.4	SS	3	6.2		111
2e3k.nb	B	/B0365-HIS ND1	B	/B0368-TYR OH	2.4	SS	3	6.1		777
2e3k.nb	D	/D0365-HIS ND1	D	/D0368-TYR OH	2.4	SS	3	5.8		2031
2ec6.nb	A	/A0584-HIS NE2	A	/A0591-TYR OH	2.4	SS	712.1			2040
2ein.nb	N	/N0261-TYR OH	N	/N0395-HIS ND1	2.4	SS	134	9.9		8198
2erv.nb	A	/A0045-TYR OH	A	/A0058-HIS ND1	2.4	SS	13	7.1		282
2erv.nb	B	/B0045-TYR OH	B	/B0058-HIS ND1	2.4	SS	-1	7.1		1071
2f7k.nb	A	/A0079-TYR OH	A	/A0246-HIS ND1	2.4	SS	16710.4			372
2fa1.nb	B	/B0116-HIS NE2	B	/B0225-TYR OH	2.4	SS	10910.0			1258
2fgj.nb	A	/A0585-HIS ND1	A	/A0595-TYR OH	2.4	SS	10	9.0		598
2fh4.nb	A	/A0464-TYR OH	A	/A0507-HIS ND1	2.4	SS	4310.3			256
2fsg.nb	B	/B0127-HIS ND1	B	/B0384-TYR OH	2.4	SS	-1	9.5		3507
2fvj.nb	A	/A0323-HIS NE2	A	/A0473-TYR OH	2.4	SS	15010.0			730
2fw4.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.4	SS	8711.6			729
2g4o.nb	D	/D0035-TYR OH	D	/D0060-HIS NE2	2.4	SS	2511.8			4366
2g67.nb	B	/B0452-HIS ND1	B	/B0461-TYR OH	2.4	SS	9	8.8		5242
2gnx.nb	A	/A0360-HIS ND1	A	/A0393-TYR OH	2.4	SS	33	9.6		845
2guw.nb	C	/C0209-TYR OH	C	/C0452-HIS ND1	2.4	SS	-1	9.0		4037
2gxa.nb	G	/G0482-HIS ND1	G	/G0532-TYR OH	2.4	SS	50	9.3		7245
2h02.nb	A	/A1815-TYR OH	A	/A1903-HIS NE2	2.4	SS	-112.1			918
2h02.nb	B	/B1815-TYR OH	B	/B1903-HIS NE2	2.4	SS	-112.1			2567
2h32.nb	A	/A0028-HIS ND1	A	/A0033-TYR OH	2.4	SS	5	8.9		121
2hij.nb	L	/L0120-HIS ND1	L	/L0166-TYR OH	2.4	SS	46	8.5		2183
2i4o.nb	C	/C0254-TYR OH	C	/C0261-HIS ND1	2.4	SS	7	9.4		4841
2i76.nb	B	/B0104-HIS ND1	B	/B0158-TYR OH	2.4	SS	-110.3			1416
2i80.nb	B	/B0017-HIS NE2	B	/B0042-TYR OH	2.4	SS	25	9.8		1682
2ibx.nb	A	/A0183-HIS ND1	A	/A0195-TYR OH	2.4	SS	1210.5			811
2ibx.nb	E	/E0183-HIS ND1	E	/E0195-TYR OH	2.4	SS	1210.5			4362
2ihi.nb	C	/C0195-HIS NE2	C	/C0205-TYR OH	2.4	SS	1011.7			3681
2ijd.nb	1	/10138-TYR OH	1	/10161-HIS ND1	2.4	SS	2310.3			556
2ioq.nb	A	/A0246-TYR OH	A	/A0265-HIS ND1	2.4	SS	19	9.5		815
2irp.nb	B	/B0174-HIS NE2	B	/B0177-TYR OH	2.4	SS	3	9.4		1996
2it4.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.4	SS	7111.2			296
2itm.nb	A	/A0259-TYR OH	A	/A0381-HIS NE2	2.4	SS	-110.5			1506
2ja6.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.4	SS	2012.7			1677
2ja6.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.4	SS	21	8.8		13788
2ja8.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.4	SS	2012.6			1687
2nvy.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.4	SS	2012.7			1857
2ny7.nb	G	/G0249-HIS ND1	G	/G0486-TYR OH	2.4	SS	-110.0			332
2nzu.nb	G	/G0223-TYR OH	G	/G0256-HIS ND1	2.4	SS	33	9.4		864
2o6b.nb	B	/B0098-TYR OH	B	/B0118-HIS ND1	2.4	SS	20	8.0		915
2o6u.nb	A	/A0098-TYR OH	A	/A0118-HIS ND1	2.4	SS	20	7.9		414
2ooe.nb	A	/A0360-HIS ND1	A	/A0381-TYR OH	2.4	SS	21	8.0		1602
2p1i.nb	E	/E0144-TYR OH	E	/E0213-HIS NE2	2.4	SS	6911.7			4775
2pc9.nb	A	/A0027-HIS ND1	A	/A0100-TYR OH	2.4	SS	7310.7			124
2pmz.nb	A	/A0433-HIS NE2	A	/A0453-TYR OH	2.4	SS	2012.7			1266
2pmz.nb	Q	/Q0433-HIS NE2	Q	/Q0453-TYR OH	2.4	SS	2012.7			12282
2pzs.nb	B	/B0461-HIS ND1	B	/B0494-TYR OH	2.4	SS	3310.5			4213
2qfx.nb	E	/E0196-HIS ND1	E	/E0237-TYR OH	2.4	SS	41	9.1		7653

2qg7.nb	A	/A0210-HIS	ND1	A	/A0394-TYR	OH	2.4	SS	-1	9.7	695
2r6c.nb	A	/A0048-HIS	NE2	A	/A0088-TYR	OH	2.4	SS	4010.3		174
2r6c.nb	C	/C0048-HIS	NE2	C	/C0088-TYR	OH	2.4	SS	4010.3		2997
2r6c.nb	E	/E0048-HIS	NE2	E	/E0088-TYR	OH	2.4	SS	4010.2		5815
2rgk.nb	B	/B0168-TYR	OH	B	/B0219-HIS	ND1	2.4	SS	51	7.6	2640
2rhs.nb	B	/B0751-TYR	OH	B	/B0755-HIS	ND1	2.4	SS	4	9.0	3907
2tun.nb	B	/B0015-HIS	ND1	B	/B0059-TYR	OH	2.4	SS	44	9.0	557
2ux0.nb	D	/D0418-TYR	OH	D	/D0444-HIS	ND1	2.4	SS	26	9.8	1780
2v0g.nb	A	/A0535-TYR	OH	A	/A0545-HIS	NE2	2.4	SS	1012.0		2267
2v8s.nb	V	/V0015-HIS	NE2	V	/V0084-TYR	OH	2.4	SS	6910.8		834
2vds.nb	A	/A0215-HIS	NE2	A	/A0280-TYR	OH	2.4	SS	6512.2		1589
2vir.nb	C	/C0183-HIS	ND1	C	/C0195-TYR	OH	2.4	SS	1210.0		2208
2vis.nb	C	/C0183-HIS	ND1	C	/C0195-TYR	OH	2.4	SS	1210.1		2197
2vn7.nb	A	/A0418-HIS	ND1	A	/A0423-TYR	OH	2.4	SS	5	7.8	2953
2vqx.nb	A	/A0036-HIS	NE2	A	/A0126-TYR	OH	2.4	SS	-111.4		200
2vsk.nb	A	/A0231-TYR	OH	A	/A0233-HIS	ND1	2.4	SS	2	7.1	179
2vum.nb	K	/K0040-HIS	ND1	K	/K0061-TYR	OH	2.4	SS	21	9.0	13866
2vv2.nb	A	/A0323-HIS	NE2	A	/A0473-TYR	OH	2.4	SS	150	9.9	549
2vyc.nb	B	/B0061-TYR	OH	B	/B0069-HIS	ND1	2.4	SS	8	8.3	3557
2vyc.nb	C	/C0061-TYR	OH	C	/C0069-HIS	ND1	2.4	SS	8	8.4	6820
2w04.nb	B	/B0437-HIS	ND1	B	/B0478-TYR	OH	2.4	SS	41	8.9	4753
2wpw.nb	A	/A0180-TYR	OH	A	/A0275-HIS	ND1	2.4	SS	-1	9.8	723
2wr1.nb	A	/A0351-TYR	OH	A	/A0440-HIS	ND1	2.4	SS	89	8.8	1420
2yw7.nb	H	/H0028-TYR	OH	H	/H0141-HIS	ND1	2.4	SS	113	9.7	4388
2zbk.nb	B	/B0099-TYR	OH	B	/B0348-HIS	NE2	2.4	SS	24911.6		1598
2zbk.nb	D	/D0099-TYR	OH	D	/D0348-HIS	NE2	2.4	SS	24911.8		4607
2zz0.nb	B	/B0403-HIS	ND1	B	/B0422-TYR	OH	2.4	SS	19	7.5	3506
3a7a.nb	A	/A0253-HIS	ND1	A	/A0302-TYR	OH	2.4	SS	4910.1		1040
3b6v.nb	B	/B0074-TYR	OH	B	/B0126-HIS	ND1	2.4	SS	5210.0		1504
3bcc.nb	B	/B0164-HIS	NE2	B	/B0316-TYR	OH	2.4	SS	13611.4		2432
3bnx.nb	A	/A0043-HIS	ND1	A	/A0126-TYR	OH	2.4	SS	83	9.4	170
3bsg.nb	A	/A0310-TYR	OH	A	/A0326-HIS	ND1	2.4	SS	16	9.6	2379
3c9m.nb	A	/A0206-TYR	OH	A	/A0211-HIS	NE2	2.4	SS	5	7.8	960
3cj5.nb	B	/B0176-TYR	OH	B	/B0562-HIS	NE2	2.4	SS	38612.2		4571
3cke.nb	A	/A0043-HIS	ND1	A	/A0126-TYR	OH	2.4	SS	83	9.2	156
3cso.nb	A	/A0103-TYR	OH	A	/A0118-HIS	ND1	2.4	SS	15	9.0	575
3cxe.nb	A	/A0367-HIS	NE2	A	/A0421-TYR	OH	2.4	SS	5410.5		1110
3da4.nb	B	/B0183-HIS	NE2	B	/B0188-TYR	OH	2.4	SS	510.1		3539
3dl5.nb	B	/B0403-HIS	ND1	B	/B0438-TYR	OH	2.4	SS	35	9.4	3702
3e1k.nb	A	/A0036-HIS	ND1	A	/A0385-TYR	OH	2.4	SS	-1	8.8	126
3e1k.nb	I	/I0036-HIS	ND1	I	/I0385-TYR	OH	2.4	SS	-1	8.9	6651
3ed1.nb	E	/E0126-HIS	NE2	E	/E0254-TYR	OH	2.4	SS	-1	9.8	5774
3f2o.nb	B	/B0098-HIS	ND1	B	/B0226-TYR	OH	2.4	SS	128	8.0	1609
3f8n.nb	A	/A0092-TYR	OH	A	/A0128-HIS	NE2	2.4	SS	3610.9		347
3f9s.nb	B	/B0035-TYR	OH	B	/B0125-HIS	ND1	2.4	SS	90	8.0	1190
3fbb.nb	E	/E0053-HIS	ND1	E	/E0058-TYR	OH	2.4	SS	5	8.2	2962
3fbe.nb	C	/C0053-HIS	ND1	C	/C0058-TYR	OH	2.4	SS	5	8.2	1591
3fy7.nb	A	/A0098-TYR	OH	A	/A0148-HIS	ND1	2.4	SS	5010.3		407
3g3s.nb	B	/B0166-HIS	ND1	B	/B0194-TYR	OH	2.4	SS	28	9.6	2980
3gbm.nb	D	/D0022-TYR	OH	D	/D0111-HIS	ND1	2.4	SS	89	8.5	3088
3ggg.nb	B	/B0147-HIS	NE2	B	/B6959-TYR	OH	2.4	SS	-112.2		3275
3glq.nb	B	/B0327-HIS	NE2	B	/B0357-TYR	OH	2.4	SS	3011.1		5286
3gnv.nb	B	/B0103-TYR	OH	B	/B0118-HIS	ND1	2.4	SS	15	9.4	3315
3goi.nb	A	/A0413-TYR	OH	A	/A0424-HIS	NE2	2.4	SS	1110.4		2087
3gtn.nb	A	/A0252-HIS	ND1	A	/A0265-TYR	OH	2.4	SS	13	9.9	1161
3gtn.nb	B	/B0252-HIS	ND1	B	/B0265-TYR	OH	2.4	SS	13	9.9	2846

3h1i.nb	B	/B0254-HIS	ND1	B	/B0325-TYR	OH	2.4	SS	71	7.4	2775
3h1i.nb	O	/O0254-HIS	ND1	O	/O0325-TYR	OH	2.4	SS	71	7.6	10520
3h1k.nb	O	/O0254-HIS	ND1	O	/O0325-TYR	OH	2.4	SS	71	7.3	10476
3h1t.nb	A	/A0428-HIS	ND1	A	/A0557-TYR	OH	2.4	SS	129	9.7	1974
3h3v.nb	B	/B0458-HIS	NE2	B	/B0478-TYR	OH	2.4	SS	2012.9		1746
3h5u.nb	A	/A0103-TYR	OH	A	/A0118-HIS	ND1	2.4	SS	15	9.1	700
3h76.nb	A	/A0228-HIS	ND1	A	/A0315-TYR	OH	2.4	SS	87	9.2	1352
3h76.nb	B	/B0228-HIS	ND1	B	/B0315-TYR	OH	2.4	SS	87	9.4	3148
3hnp.nb	C	/C0018-HIS	ND1	C	/C0305-TYR	OH	2.4	SS	-1	8.8	2895
3hou.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.4	SS	2012.8		1779
3hov.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.4	SS	2013.0		1784
3how.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.4	SS	2013.0		1708
3hox.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.4	SS	2013.2		1759
3hoy.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.4	SS	2012.9		1762
3hoy.nb	A	/A0804-TYR	OH	A	/A0816-HIS	NE2	2.4	SS	1211.3		3099
3hoz.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.4	SS	2013.1		1760
3hoz.nb	K	/K0040-HIS	ND1	K	/K0061-TYR	OH	2.4	SS	21	8.9	14418
3hri.nb	C	/C0075-HIS	ND1	C	/C0148-TYR	OH	2.4	SS	-1	8.7	3169
3hx1.nb	A	/A0012-HIS	ND1	A	/A0112-TYR	OH	2.4	SS	-1	7.4	22
3i23.nb	A	/A0018-HIS	ND1	A	/A0305-TYR	OH	2.4	SS	287	9.0	123
3i3r.nb	A	/A0394-HIS	ND1	A	/A0428-TYR	OH	2.4	SS	34	9.7	1894
3i4m.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.4	SS	2012.7		1816
3i4n.nb	K	/K0040-HIS	ND1	K	/K0061-TYR	OH	2.4	SS	21	9.1	14363
3i9v.nb	1	/10038-TYR	OH	1	/10112-HIS	ND1	2.4	SS	74	8.4	161
3i9v.nb	A	/A0038-TYR	OH	A	/A0112-HIS	ND1	2.4	SS	74	8.4	9365
3ias.nb	1	/10038-TYR	OH	1	/10112-HIS	ND1	2.4	SS	74	8.2	167
3ias.nb	A	/A0038-TYR	OH	A	/A0112-HIS	ND1	2.4	SS	74	8.2	9420
3ib3.nb	A	/A0373-HIS	NE2	A	/A0397-TYR	OH	2.4	SS	24	9.5	2459
3inb.nb	A	/A0529-TYR	OH	A	/A0536-HIS	ND1	2.4	SS	7	7.5	1185
3kcg.nb	H	/H0185-HIS	ND1	H	/H0225-TYR	OH	2.4	SS	41	7.3	1488
3kcq.nb	D	/D0101-HIS	NE2	D	/D0139-TYR	OH	2.4	SS	38	7.6	3296
3l06.nb	A	/A0155-HIS	NE2	A	/A0173-TYR	OH	2.4	SS	1812.2		778
3l72.nb	B	/B0254-HIS	ND1	B	/B0325-TYR	OH	2.4	SS	71	7.2	2822
3l73.nb	B	/B0254-HIS	ND1	B	/B0325-TYR	OH	2.4	SS	71	7.3	2800
3lc3.nb	A	/A0185-HIS	ND1	A	/A0225-TYR	OH	2.4	SS	41	8.0	1128
3lc3.nb	C	/C0185-HIS	ND1	C	/C0225-TYR	OH	2.4	SS	41	7.9	2813
4cox.nb	A	/A0234-TYR	OH	A	/A0309-HIS	ND1	2.4	SS	75	9.8	944
4cox.nb	B	/B0234-TYR	OH	B	/B0309-HIS	ND1	2.4	SS	75	9.8	3314
4cox.nb	C	/C0234-TYR	OH	C	/C0309-HIS	ND1	2.4	SS	75	9.8	5694
4cox.nb	D	/D0234-TYR	OH	D	/D0309-HIS	ND1	2.4	SS	75	9.7	8077
5cac.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.4	SS	8611.8		684
5cox.nb	B	/B0234-TYR	OH	B	/B0309-HIS	ND1	2.4	SS	7510.1		3245
5cox.nb	C	/C0133-HIS	ND1	C	/C0147-TYR	OH	2.4	SS	14	9.1	5089
7gpb.nb	B	/B0571-HIS	ND1	B	/B0613-TYR	OH	2.4	SS	42	8.5	6077
12ca.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7112.0		276
16vp.nb	A	/A0168-TYR	OH	A	/A0229-HIS	ND1	2.5	SS	61	9.5	825
1a19.nb	B	/B0017-HIS	ND1	B	/B0030-TYR	OH	2.5	SS	13	8.6	432
1a9y.nb	A	/A0177-TYR	OH	A	/A0243-HIS	NE2	2.5	SS	6610.9		1410
1air.nb	A	/A0228-HIS	ND1	A	/A0320-TYR	OH	2.5	SS	9210.8		1402
1ajm.nb	A	/A0147-HIS	ND1	A	/A0181-TYR	OH	2.5	SS	34	9.6	766
1aqx.nb	C	/C0118-TYR	OH	C	/C0162-HIS	NE2	2.5	SS	4410.7		2938
1ati.nb	B	/B0076-TYR	OH	B	/B0337-HIS	ND1	2.5	SS	-1	9.6	2145
1avn.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7		705
1ay0.nb	B	/B0079-HIS	NE2	B	/B0294-TYR	OH	2.5	SS	215	9.6	3296
1b65.nb	B	/B0235-HIS	NE2	B	/B0371-TYR	OH	2.5	SS	-111.8		2476
1b65.nb	C	/C0235-HIS	NE2	C	/C0371-TYR	OH	2.5	SS	-111.8		3933

1b65.nb	D	/D0235-HIS	NE2	D	/D0371-TYR	OH	2.5	SS	-111.8	5395
1b6r.nb	A	/A0305-TYR	OH	A	/A0317-HIS	ND1	2.5	SS	12 8.3	1443
1b6s.nb	A	/A0305-TYR	OH	A	/A0317-HIS	ND1	2.5	SS	12 8.3	1213
1b7z.nb	A	/A0192-TYR	OH	A	/A0253-HIS	NE2	2.5	SS	6112.7	951
1b94.nb	A	/A0072-TYR	OH	A	/A0131-HIS	ND1	2.5	SS	5910.4	385
1b9c.nb	C	/C0074-TYR	OH	C	/C0199-HIS	NE2	2.5	SS	12510.5	2594
1b9c.nb	D	/D0074-TYR	OH	D	/D0199-HIS	NE2	2.5	SS	12510.5	3823
1bcc.nb	B	/B0164-HIS	NE2	B	/B0316-TYR	OH	2.5	SS	13611.5	2400
1be3.nb	B	/B0254-HIS	ND1	B	/B0325-TYR	OH	2.5	SS	71 7.3	2714
1bgy.nb	B	/B0254-HIS	ND1	B	/B0325-TYR	OH	2.5	SS	71 7.3	2737
1bka.nb	A	/A0192-TYR	OH	A	/A0253-HIS	NE2	2.5	SS	6113.0	1016
1bn3.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7111.7	321
1bpo.nb	A	/A0129-HIS	NE2	A	/A0156-TYR	OH	2.5	SS	2711.3	543
1bpo.nb	B	/B0129-HIS	NE2	B	/B0156-TYR	OH	2.5	SS	2711.2	2456
1bqc.nb	A	/A0044-HIS	ND1	A	/A0286-TYR	OH	2.5	SS	242 8.6	431
1br2.nb	D	/D0585-HIS	NE2	D	/D0592-TYR	OH	2.5	SS	711.5	10974
1br4.nb	A	/A0585-HIS	NE2	A	/A0592-TYR	OH	2.5	SS	712.2	2346
1br4.nb	C	/C0585-HIS	NE2	C	/C0592-TYR	OH	2.5	SS	712.2	5988
1br4.nb	E	/E0585-HIS	NE2	E	/E0592-TYR	OH	2.5	SS	712.2	9636
1br4.nb	G	/G0585-HIS	NE2	G	/G0592-TYR	OH	2.5	SS	712.2	13270
1bt4.nb	A	/A0147-HIS	NE2	A	/A0192-TYR	OH	2.5	SS	4510.9	815
1c2t.nb	B	/B0054-HIS	NE2	B	/B0078-TYR	OH	2.5	SS	2411.8	1456
1c3e.nb	A	/A0054-HIS	NE2	A	/A0078-TYR	OH	2.5	SS	2411.8	329
1c3e.nb	B	/B0054-HIS	NE2	B	/B0078-TYR	OH	2.5	SS	2411.8	1460
1c3x.nb	B	/B0154-HIS	ND1	B	/B0175-TYR	OH	2.5	SS	21 8.9	2063
1c5x.nb	B	/B0094-TYR	OH	B	/B0099-HIS	ND1	2.5	SS	7 7.1	642
1c5y.nb	B	/B0094-TYR	OH	B	/B0099-HIS	ND1	2.5	SS	7 7.0	639
1c5z.nb	B	/B0094-TYR	OH	B	/B0099-HIS	ND1	2.5	SS	7 7.0	616
1ca2.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7	705
1ca3.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7111.9	285
1ccs.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7	671
1cct.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7111.9	296
1ccu.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.6	675
1cia.nb	A	/A0144-HIS	NE2	A	/A0168-TYR	OH	2.5	SS	2411.1	806
1cla.nb	A	/A0144-HIS	NE2	A	/A0168-TYR	OH	2.5	SS	2411.1	858
1cnk.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7111.8	330
1cny.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7	641
1cq6.nb	A	/A0161-TYR	OH	A	/A0166-HIS	ND1	2.5	SS	5 7.0	745
1csj.nb	B	/B0103-TYR	OH	B	/B0118-HIS	ND1	2.5	SS	15 9.2	2957
1cva.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7	654
1cvc.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7112.0	292
1cvc.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7	660
1cve.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.6	706
1cvf.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7112.0	293
1cvh.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7111.9	275
1cvh.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7	654
1cx2.nb	A	/A0234-TYR	OH	A	/A0309-HIS	ND1	2.5	SS	7510.1	932
1cx2.nb	C	/C0234-TYR	OH	C	/C0309-HIS	ND1	2.5	SS	7510.1	5661
1cx2.nb	D	/D0234-TYR	OH	D	/D0309-HIS	ND1	2.5	SS	7510.1	8034
1d09.nb	A	/A0156-HIS	ND1	A	/A0185-TYR	OH	2.5	SS	29 7.7	830
1d0x.nb	A	/A0572-HIS	NE2	A	/A0579-TYR	OH	2.5	SS	711.9	3828
1d1c.nb	A	/A0572-HIS	NE2	A	/A0579-TYR	OH	2.5	SS	711.9	3502
1dbh.nb	A	/A0349-HIS	NE2	A	/A0353-TYR	OH	2.5	SS	4 6.7	839
1dbz.nb	A	/A0189-TYR	OH	A	/A0278-HIS	ND1	2.5	SS	89 9.4	618
1dbz.nb	B	/B0189-TYR	OH	B	/B0278-HIS	ND1	2.5	SS	89 9.3	1908
1dd1.nb	B	/B0290-HIS	ND1	B	/B0430-TYR	OH	2.5	SS	-1 7.6	1155

1de8.nb	B	/B0151-HIS ND1	B	/B0184-TYR OH	2.5	SS	3310.0		505
1dgk.nb	N	/N0417-TYR OH	N	/N0428-HIS NE2	2.5	SS	1110.6		1919
1diy.nb	A	/A0234-TYR OH	A	/A0309-HIS ND1	2.5	SS	7510.1		1025
1dma.nb	A	/A0426-HIS ND1	A	/A0502-TYR OH	2.5	SS	-1	9.2	119
1dp4.nb	A	/A0141-HIS NE2	A	/A0211-TYR OH	2.5	SS	7012.3		961
1dtw.nb	A	/A0202-HIS ND1	A	/A0246-TYR OH	2.5	SS	44	8.9	940
1du4.nb	A	/A0021-TYR OH	A	/A0145-HIS ND1	2.5	SS	124	9.3	160
1dua.nb	A	/A0010-HIS ND1	A	/A0187-TYR OH	2.5	SS	177	9.1	40
1due.nb	A	/A0010-HIS ND1	A	/A0187-TYR OH	2.5	SS	177	9.2	41
1dva.nb	I	/I0101-HIS ND1	I	/I0234-TYR OH	2.5	SS	-1	8.8	1750
1e2m.nb	A	/A0058-HIS ND1	A	/A0172-TYR OH	2.5	SS	-110.3		113
1e5l.nb	A	/A0131-HIS ND1	A	/A0233-TYR OH	2.5	SS	102	8.5	650
1e5r.nb	B	/B0022-TYR OH	B	/B0071-HIS ND1	2.5	SS	-1	8.8	1519
1e6i.nb	A	/A0332-HIS ND1	A	/A0434-TYR OH	2.5	SS	102	9.9	19
1e8g.nb	A	/A0149-HIS ND1	A	/A0408-TYR OH	2.5	SS	25910.1		776
1e8g.nb	B	/B0149-HIS ND1	B	/B0408-TYR OH	2.5	SS	25910.1		3752
1e8t.nb	B	/B0187-TYR OH	B	/B0189-HIS ND1	2.5	SS	2	7.1	2764
1ebb.nb	A	/A0053-TYR OH	A	/A0141-HIS NE2	2.5	SS	8811.6		312
1ebv.nb	A	/A0234-TYR OH	A	/A0309-HIS ND1	2.5	SS	7510.1		915
1emf.nb	A	/A0074-TYR OH	A	/A0199-HIS NE2	2.5	SS	12510.9		408
1eou.nb	A	/A0107-HIS NE2	A	/A0193-TYR OH	2.5	SS	8611.7		720
1ep8.nb	B	/B0083-HIS ND1	B	/B0085-TYR OH	2.5	SS	2	6.4	901
1eqy.nb	S	/S0062-HIS NE2	S	/S0109-TYR OH	2.5	SS	4711.0		445
1eth.nb	A	/A0271-TYR OH	A	/A0310-HIS ND1	2.5	SS	39	6.1	1238
1ex5.nb	B	/B0080-HIS ND1	B	/B0137-TYR OH	2.5	SS	57	9.3	1823
1f1r.nb	B	/B0248-HIS NE2	B	/B0257-TYR OH	2.5	SS	911.8		3432
1f30.nb	A	/A0107-TYR OH	A	/A0117-HIS ND1	2.5	SS	10	9.2	432
1f30.nb	B	/B0107-TYR OH	B	/B0117-HIS ND1	2.5	SS	10	9.2	1105
1f30.nb	D	/D0107-TYR OH	D	/D0117-HIS ND1	2.5	SS	10	9.2	2447
1f30.nb	E	/E0107-TYR OH	E	/E0117-HIS ND1	2.5	SS	10	9.2	3116
1f30.nb	G	/G0107-TYR OH	G	/G0117-HIS ND1	2.5	SS	10	9.2	4461
1f30.nb	I	/I0107-TYR OH	I	/I0117-HIS ND1	2.5	SS	10	9.2	5808
1f30.nb	J	/J0107-TYR OH	J	/J0117-HIS ND1	2.5	SS	10	9.2	6480
1f30.nb	K	/K0107-TYR OH	K	/K0117-HIS ND1	2.5	SS	10	9.2	7151
1f30.nb	L	/L0107-TYR OH	L	/L0117-HIS ND1	2.5	SS	10	9.2	7824
1f37.nb	B	/B0074-TYR OH	B	/B0089-HIS ND1	2.5	SS	1511.4		843
1f4e.nb	A	/A0147-HIS ND1	A	/A0181-TYR OH	2.5	SS	34	9.6	1038
1f4f.nb	B	/B0147-HIS ND1	B	/B0181-TYR OH	2.5	SS	34	9.7	2759
1f5q.nb	D	/D0043-HIS ND1	D	/D0048-TYR OH	2.5	SS	5	8.3	3926
1f8m.nb	A	/A0089-TYR OH	A	/A0180-HIS NE2	2.5	SS	9110.6		407
1fba.nb	D	/D0080-HIS ND1	D	/D0137-TYR OH	2.5	SS	57	9.3	4984
1fbd.nb	A	/A0279-TYR OH	A	/A0311-HIS ND1	2.5	SS	32	8.4	1066
1fcm.nb	A	/A0311-HIS ND1	A	/A0322-TYR OH	2.5	SS	11	7.4	1513
1fco.nb	B	/B0311-HIS ND1	B	/B0322-TYR OH	2.5	SS	11	7.6	3408
1fea.nb	C	/C0039-HIS ND1	C	/C0182-TYR OH	2.5	SS	14310.5		4147
1feb.nb	B	/B0039-HIS ND1	B	/B0182-TYR OH	2.5	SS	14310.4		2787
1fgm.nb	A	/A0290-HIS ND1	A	/A0293-TYR OH	2.5	SS	3	6.0	1808
1fgq.nb	A	/A0290-HIS ND1	A	/A0293-TYR OH	2.5	SS	3	6.0	1796
1fj6.nb	A	/A0279-TYR OH	A	/A0311-HIS ND1	2.5	SS	32	8.4	1374
1fkn.nb	A	/A0181-HIS ND1	A	/A0184-TYR OH	2.5	SS	3	6.2	1213
1fnc.nb	A	/A0059-HIS ND1	A	/A0212-TYR OH	2.5	SS	153	9.6	288
1fnn.nb	A	/A0288-HIS ND1	A	/A0317-TYR OH	2.5	SS	29	9.1	1621
1fp9.nb	A	/A0379-HIS ND1	A	/A0417-TYR OH	2.5	SS	3810.5		1708
1fpk.nb	A	/A0279-TYR OH	A	/A0311-HIS ND1	2.5	SS	32	8.4	1066
1frn.nb	A	/A0059-HIS ND1	A	/A0212-TYR OH	2.5	SS	153	9.6	283
1frq.nb	A	/A0059-HIS ND1	A	/A0212-TYR OH	2.5	SS	153	9.7	281

1fsn.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.6		663
1fsn.nb	B	/B0107-HIS NE2	B	/B0194-TYR OH	2.5	SS	8611.6		2031
1fsr.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.6		571
1fsr.nb	B	/B0107-HIS NE2	B	/B0194-TYR OH	2.5	SS	8611.6		1732
1fug.nb	A	/A0276-TYR OH	A	/A0359-HIS NE2	2.5	SS	83	9.1	1100
1g71.nb	B	/B0142-HIS ND1	B	/B0307-TYR OH	2.5	SS	165	7.7	2872
1g88.nb	B	/B0290-HIS ND1	B	/B0430-TYR OH	2.5	SS	-1	7.7	875
1gfl.nb	A	/A0074-TYR OH	A	/A0199-HIS NE2	2.5	SS	12510.7		518
1ggm.nb	B	/B0076-TYR OH	B	/B0337-HIS ND1	2.5	SS	-1	9.0	2160
1gi7.nb	B	/B0094-TYR OH	B	/B0099-HIS ND1	2.5	SS	7	7.0	652
1gi8.nb	B	/B0094-TYR OH	B	/B0099-HIS ND1	2.5	SS	7	6.9	665
1gk0.nb	B	/B0224-HIS NE2	B	/B0264-TYR OH	2.5	SS	4011.6		1584
1gk1.nb	B	/B0224-HIS NE2	B	/B0264-TYR OH	2.5	SS	4011.8		1560
1gpa.nb	C	/C0571-HIS ND1	C	/C0613-TYR OH	2.5	SS	42	8.8	9482
1grc.nb	B	/B0054-HIS NE2	B	/B0078-TYR OH	2.5	SS	2411.9		1013
1gsy.nb	A	/A0118-TYR OH	A	/A0162-HIS NE2	2.5	SS	-111.1		629
1gt8.nb	A	/A0211-TYR OH	A	/A0504-HIS ND1	2.5	SS	293	8.9	1010
1gth.nb	A	/A0211-TYR OH	A	/A0504-HIS ND1	2.5	SS	293	8.8	996
1gth.nb	C	/C0211-TYR OH	C	/C0504-HIS ND1	2.5	SS	293	8.9	9151
1gwc.nb	A	/A0061-HIS ND1	A	/A0075-TYR OH	2.5	SS	1410.1		447
1gwc.nb	B	/B0061-HIS ND1	B	/B0075-TYR OH	2.5	SS	1410.1		1906
1gwc.nb	C	/C0061-HIS ND1	C	/C0075-TYR OH	2.5	SS	1410.2		3371
1gy8.nb	A	/A0200-TYR OH	A	/A0280-HIS NE2	2.5	SS	-110.8		868
1gy8.nb	B	/B0200-TYR OH	B	/B0280-HIS NE2	2.5	SS	-110.8		2397
1gy8.nb	D	/D0200-TYR OH	D	/D0280-HIS NE2	2.5	SS	-110.8		5442
1gyt.nb	B	/B0123-TYR OH	B	/B0176-HIS ND1	2.5	SS	53	9.7	2690
1gyt.nb	D	/D0123-TYR OH	D	/D0176-HIS ND1	2.5	SS	53	9.9	6975
1h0h.nb	K	/K0670-TYR OH	K	/K0681-HIS ND1	2.5	SS	11	9.4	8528
1h5n.nb	C	/C0146-TYR OH	C	/C0439-HIS ND1	2.5	SS	-1	9.1	4097
1h5y.nb	A	/A0042-TYR OH	A	/A0231-HIS ND1	2.5	SS	189	9.8	293
1h5y.nb	B	/B0042-TYR OH	B	/B0231-HIS ND1	2.5	SS	189	9.8	1792
1hc1.nb	C	/C0262-TYR OH	C	/C0370-HIS NE2	2.5	SS	10811.6		6310
1hc1.nb	C	/C0302-HIS ND1	C	/C0304-TYR OH	2.5	SS	2	5.4	6465
1hc1.nb	D	/D0262-TYR OH	D	/D0370-HIS NE2	2.5	SS	10811.6		8877
1hc1.nb	E	/E0262-TYR OH	E	/E0370-HIS NE2	2.5	SS	10811.6		11437
1hc1.nb	F	/F0262-TYR OH	F	/F0370-HIS NE2	2.5	SS	10811.5		14006
1hea.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.8		664
1hk7.nb	A	/A0289-TYR OH	A	/A0308-HIS ND1	2.5	SS	19	9.5	92
1hkq.nb	A	/A0045-TYR OH	A	/A0097-HIS ND1	2.5	SS	52	8.8	182
1hlb.nb	A	/A0104-HIS ND1	A	/A0114-TYR OH	2.5	SS	1010.3		598
1hr6.nb	A	/A0159-HIS NE2	A	/A0323-TYR OH	2.5	SS	16411.8		704
1hr6.nb	D	/D0167-HIS NE2	D	/D0330-TYR OH	2.5	SS	16312.0		6265
1hr6.nb	G	/G0159-HIS NE2	G	/G0323-TYR OH	2.5	SS	16411.8		11762
1hr8.nb	D	/D0167-HIS NE2	D	/D0330-TYR OH	2.5	SS	16312.1		6192
1hr8.nb	F	/F0167-HIS NE2	F	/F0330-TYR OH	2.5	SS	16312.2		9834
1hr9.nb	A	/A0159-HIS NE2	A	/A0323-TYR OH	2.5	SS	-111.7		693
1hr9.nb	D	/D0167-HIS NE2	D	/D0330-TYR OH	2.5	SS	16312.0		6172
1hr9.nb	E	/E0159-HIS NE2	E	/E0323-TYR OH	2.5	SS	-111.7		7983
1hr9.nb	F	/F0167-HIS NE2	F	/F0330-TYR OH	2.5	SS	16312.2		9813
1hu9.nb	A	/A0590-TYR OH	A	/A0676-HIS ND1	2.5	SS	8610.4		3215
1huh.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8711.6		726
1hw6.nb	A	/A0165-HIS ND1	A	/A0195-TYR OH	2.5	SS	3010.7		1073
1hzj.nb	B	/B0185-TYR OH	B	/B0251-HIS NE2	2.5	SS	6610.7		4001
1i3l.nb	B	/B0185-TYR OH	B	/B0251-HIS NE2	2.5	SS	6610.9		3890
1i3q.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.9		1763
1i6h.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.5	SS	8	9.9	10234

1i7k.nb	B	/B0103-TYR OH	B	/B0151-HIS ND1	2.5	SS	48	9.4		1207
1i8z.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.5	SS	7111.7			346
1i8z.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.5			735
1i9r.nb	B	/B0125-HIS ND1	B	/B0172-TYR OH	2.5	SS	47	9.2		520
1ilg.nb	A	/A0242-HIS NE2	A	/A0306-TYR OH	2.5	SS	6411.7			470
1imv.nb	A	/A0099-HIS ND1	A	/A0142-TYR OH	2.5	SS	43	7.9		479
1iqa.nb	A	/A0166-HIS ND1	A	/A0216-TYR OH	2.5	SS	50	9.1		35
1iri.nb	B	/B0344-TYR OH	B	/B0414-HIS NE2	2.5	SS	7010.9			3951
1iri.nb	D	/D0344-TYR OH	D	/D0414-HIS NE2	2.5	SS	7010.9			8638
1j0b.nb	A	/A0080-HIS ND1	A	/A0317-TYR OH	2.5	SS	237	9.8		400
1j0b.nb	C	/C0080-HIS NE2	C	/C0256-TYR OH	2.5	SS	17611.8			3114
1j0b.nb	I	/I0080-HIS ND1	I	/I0317-TYR OH	2.5	SS	237	9.2		11149
1j0b.nb	I	/I0080-HIS NE2	I	/I0256-TYR OH	2.5	SS	17611.4			11147
1j0k.nb	A	/A0207-TYR OH	A	/A0423-HIS NE2	2.5	SS	21611.8			974
1j3b.nb	B	/B0027-HIS ND1	B	/B0100-TYR OH	2.5	SS	7310.6			3415
1ja0.nb	B	/B0302-HIS ND1	B	/B0575-TYR OH	2.5	SS	-1	9.0		3247
1ja0.nb	B	/B0392-TYR OH	B	/B0443-HIS ND1	2.5	SS	5110.5			3712
1jc0.nb	B	/B0074-TYR OH	B	/B0199-HIS NE2	2.5	SS	12510.7			1551
1jh5.nb	A	/A0060-TYR OH	A	/A0069-HIS ND1	2.5	SS	9	9.8		288
1jh5.nb	B	/B0060-TYR OH	B	/B0069-HIS ND1	2.5	SS	9	9.8		802
1jh5.nb	C	/C0060-TYR OH	C	/C0069-HIS ND1	2.5	SS	9	9.8		1319
1jh5.nb	D	/D0060-TYR OH	D	/D0069-HIS ND1	2.5	SS	9	9.8		1832
1jh5.nb	E	/E0060-TYR OH	E	/E0069-HIS ND1	2.5	SS	9	9.8		2344
1jh5.nb	F	/F0060-TYR OH	F	/F0069-HIS ND1	2.5	SS	9	9.8		2857
1jh5.nb	G	/G0060-TYR OH	G	/G0069-HIS ND1	2.5	SS	9	9.8		3369
1jh5.nb	H	/H0060-TYR OH	H	/H0069-HIS ND1	2.5	SS	9	9.8		3882
1jh5.nb	I	/I0060-TYR OH	I	/I0069-HIS ND1	2.5	SS	9	9.8		4396
1jh5.nb	J	/J0060-TYR OH	J	/J0069-HIS ND1	2.5	SS	9	9.8		4910
1ji3.nb	A	/A0029-TYR OH	A	/A0112-HIS ND1	2.5	SS	8310.2			214
1ji3.nb	B	/B0029-TYR OH	B	/B0112-HIS ND1	2.5	SS	8310.2			2418
1jiq.nb	D	/D0344-TYR OH	D	/D0414-HIS NE2	2.5	SS	7010.9			8775
1jj7.nb	A	/A0622-HIS ND1	A	/A0632-TYR OH	2.5	SS	10	8.6		780
1jnf.nb	A	/A0188-TYR OH	A	/A0249-HIS NE2	2.5	SS	6112.6			1120
1jqo.nb	A	/A0462-HIS NE2	A	/A0532-TYR OH	2.5	SS	7012.2			1930
1jre.nb	C	/C0107-TYR OH	C	/C0117-HIS ND1	2.5	SS	10	9.4		1789
1jre.nb	F	/F0107-TYR OH	F	/F0117-HIS ND1	2.5	SS	10	9.4		3808
1jre.nb	H	/H0107-TYR OH	H	/H0117-HIS ND1	2.5	SS	10	9.4		5153
1js6.nb	A	/A0020-TYR OH	A	/A0070-HIS ND1	2.5	SS	5010.4			93
1js6.nb	B	/B0020-TYR OH	B	/B0070-HIS ND1	2.5	SS	5010.4			2227
1js8.nb	B	/B2648-TYR OH	B	/B2785-HIS NE2	2.5	SS	13712.6			3015
1jsm.nb	B	/B0022-TYR OH	B	/B0111-HIS ND1	2.5	SS	89	8.7		1985
1jsn.nb	A	/A0179-HIS ND1	A	/A0191-TYR OH	2.5	SS	1210.4			1099
1jts.nb	A	/A0107-TYR OH	A	/A0117-HIS ND1	2.5	SS	10	9.5		434
1jts.nb	E	/E0107-TYR OH	E	/E0117-HIS ND1	2.5	SS	10	9.3		3136
1jts.nb	F	/F0107-TYR OH	F	/F0117-HIS ND1	2.5	SS	10	9.5		3816
1jts.nb	I	/I0107-TYR OH	I	/I0117-HIS ND1	2.5	SS	10	9.4		5830
1jts.nb	O	/O0107-TYR OH	O	/O0117-HIS ND1	2.5	SS	10	9.4		9909
1jts.nb	R	/R0107-TYR OH	R	/R0117-HIS ND1	2.5	SS	10	9.4		11942
1jts.nb	S	/S0107-TYR OH	S	/S0117-HIS ND1	2.5	SS	10	9.5		12616
1jts.nb	W	/W0107-TYR OH	W	/W0117-HIS ND1	2.5	SS	10	9.3		15319
1jut.nb	B	/B0147-HIS ND1	B	/B0181-TYR OH	2.5	SS	34	9.7		1997
1jxz.nb	B	/B0150-TYR OH	B	/B0218-HIS ND1	2.5	SS	6810.3			2781
1jz5.nb	D	/D0357-HIS ND1	D	/D0392-TYR OH	2.5	SS	35	8.8		14112
1k1w.nb	A	/A0212-HIS ND1	A	/A0252-TYR OH	2.5	SS	-111.0			1090
1k1y.nb	B	/B0358-HIS NE2	B	/B0443-TYR OH	2.5	SS	8511.5			4372
1k20.nb	B	/B0031-TYR OH	B	/B0132-HIS NE2	2.5	SS	101	9.4		2524

1k28.nb	D	/D0113-HIS	ND1	D	/D0140-TYR	OH	2.5	SS	27	8.2	2849
1k83.nb	C	/C0180-TYR	OH	C	/C0188-HIS	ND1	2.5	SS	8	9.8	10352
1k8t.nb	A	/A0311-HIS	ND1	A	/A0492-TYR	OH	2.5	SS	18110.2		107
1kbu.nb	A	/A0074-TYR	OH	A	/A0091-HIS	ND1	2.5	SS	17	9.5	287
1khv.nb	A	/A0321-HIS	NE2	A	/A0358-TYR	OH	2.5	SS	3711.3		1575
1khw.nb	A	/A0166-HIS	NE2	A	/A0168-TYR	OH	2.5	SS	2	6.9	767
1khw.nb	A	/A0321-HIS	NE2	A	/A0358-TYR	OH	2.5	SS	3711.4		1424
1ki6.nb	A	/A0058-HIS	ND1	A	/A0172-TYR	OH	2.5	SS	-110.3		102
1kit.nb	A	/A0447-TYR	OH	A	/A0452-HIS	ND1	2.5	SS	5	7.4	2672
1kku.nb	A	/A0065-HIS	ND1	A	/A0247-TYR	OH	2.5	SS	-1	9.0	326
1kmp.nb	A	/A0610-TYR	OH	A	/A0634-HIS	ND1	2.5	SS	24	7.5	2750
1ko9.nb	A	/A0013-HIS	NE2	A	/A0178-TYR	OH	2.5	SS	16511.4		14
1kpg.nb	B	/B0016-TYR	OH	B	/B0141-HIS	NE2	2.5	SS	12511.9		1845
1kpg.nb	C	/C0016-TYR	OH	C	/C0141-HIS	NE2	2.5	SS	12511.8		3543
1kvt.nb	A	/A0177-TYR	OH	A	/A0243-HIS	NE2	2.5	SS	6610.9		1209
1kyq.nb	B	/B0009-HIS	ND1	B	/B0108-TYR	OH	2.5	SS	9910.0		1439
1kz7.nb	A	/A0693-HIS	NE2	A	/A0725-TYR	OH	2.5	SS	3211.7		403
1kz7.nb	C	/C1814-HIS	ND1	C	/C1889-TYR	OH	2.5	SS	-1	8.0	3727
1kzg.nb	A	/A0693-HIS	NE2	A	/A0725-TYR	OH	2.5	SS	3211.9		376
1kzg.nb	C	/C1693-HIS	NE2	C	/C1725-TYR	OH	2.5	SS	3211.9		2771
1l0l.nb	A	/A0152-TYR	OH	A	/A0243-HIS	ND1	2.5	SS	91	9.0	725
1l0n.nb	A	/A0152-TYR	OH	A	/A0243-HIS	ND1	2.5	SS	91	9.0	725
1l0n.nb	A	/A0154-HIS	NE2	A	/A0314-TYR	OH	2.5	SS	16011.6		740
1l0n.nb	A	/A0279-HIS	ND1	A	/A0284-TYR	OH	2.5	SS	5	9.7	1221
1l1n.nb	A	/A0138-TYR	OH	A	/A0161-HIS	ND1	2.5	SS	23	9.9	759
1l5g.nb	B	/B0115-TYR	OH	B	/B0192-HIS	ND1	2.5	SS	7710.2		3729
1l8h.nb	B	/B0107-TYR	OH	B	/B0117-HIS	ND1	2.5	SS	10	9.4	1092
1l8h.nb	D	/D0107-TYR	OH	D	/D0117-HIS	ND1	2.5	SS	10	9.4	2432
1l8h.nb	H	/H0107-TYR	OH	H	/H0117-HIS	ND1	2.5	SS	10	9.4	5094
1l8h.nb	K	/K0107-TYR	OH	K	/K0117-HIS	ND1	2.5	SS	10	9.4	7097
1l8h.nb	L	/L0107-TYR	OH	L	/L0117-HIS	ND1	2.5	SS	10	9.4	7756
1l8i.nb	C	/C0107-TYR	OH	C	/C0117-HIS	ND1	2.5	SS	10	9.5	1745
1l9e.nb	A	/A0055-TYR	OH	A	/A0345-HIS	ND1	2.5	SS	29010.7		404
1lb1.nb	A	/A0693-HIS	NE2	A	/A0725-TYR	OH	2.5	SS	3211.8		370
1lb1.nb	C	/C0693-HIS	NE2	C	/C0725-TYR	OH	2.5	SS	3211.9		2470
1lb1.nb	E	/E0693-HIS	NE2	E	/E0725-TYR	OH	2.5	SS	3211.8		4563
1ldj.nb	A	/A0343-HIS	NE2	A	/A0377-TYR	OH	2.5	SS	34	9.9	1232
1ldj.nb	A	/A0727-HIS	ND1	A	/A0772-TYR	OH	2.5	SS	45	7.5	2865
1led.nb	A	/A0073-TYR	OH	A	/A0175-HIS	ND1	2.5	SS	102	7.2	436
1lev.nb	A	/A0279-TYR	OH	A	/A0311-HIS	ND1	2.5	SS	32	8.4	1296
1lkx.nb	A	/A0507-HIS	NE2	A	/A0514-TYR	OH	2.5	SS	711.6		2172
1lkx.nb	B	/B0507-HIS	NE2	B	/B0514-TYR	OH	2.5	SS	711.6		4900
1lkx.nb	C	/C0507-HIS	NE2	C	/C0514-TYR	OH	2.5	SS	711.6		7616
1lkx.nb	D	/D0507-HIS	NE2	D	/D0514-TYR	OH	2.5	SS	711.6		10448
1llw.nb	A	/A1007-HIS	ND1	A	/A1010-TYR	OH	2.5	SS	3	7.1	4309
1lyv.nb	A	/A0301-TYR	OH	A	/A0402-HIS	NE2	2.5	SS	10113.0		961
1m06.nb	F	/F0109-TYR	OH	F	/F0125-HIS	ND1	2.5	SS	16	8.5	553
1m57.nb	A	/A0437-TYR	OH	A	/A0456-HIS	ND1	2.5	SS	1910.9		2004
1m8q.nb	A	/A0583-HIS	NE2	A	/A0590-TYR	OH	2.5	SS	712.0		2465
1m8q.nb	D	/D0583-HIS	NE2	D	/D0590-TYR	OH	2.5	SS	712.0		6708
1m8q.nb	G	/G0583-HIS	NE2	G	/G0590-TYR	OH	2.5	SS	712.0		10797
1m8q.nb	P	/P0583-HIS	NE2	P	/P0590-TYR	OH	2.5	SS	712.0		14895
1m8v.nb	A	/A0110-HIS	ND1	A	/A0134-TYR	OH	2.5	SS	24	8.1	38
1m8v.nb	D	/D0410-HIS	ND1	D	/D0434-TYR	OH	2.5	SS	24	8.2	840
1m8v.nb	I	/I0210-HIS	ND1	I	/I0234-TYR	OH	2.5	SS	24	8.1	2201
1m8v.nb	M	/M0610-HIS	ND1	M	/M0634-TYR	OH	2.5	SS	24	8.3	3255

1maw.nb	D	/D0125-TYR OH	D	/D0150-HIS NE2	2.5	SS	2510.2			4547
1mdz.nb	A	/A0068-HIS ND1	A	/A0242-TYR OH	2.5	SS	-1	9.9		459
1mmd.nb	A	/A0572-HIS NE2	A	/A0579-TYR OH	2.5	SS	711.8			3367
1mqm.nb	D	/D0183-HIS ND1	D	/D0195-TYR OH	2.5	SS	1210.3			2559
1mqn.nb	D	/D0183-HIS ND1	D	/D0195-TYR OH	2.5	SS	1210.3			2559
1n38.nb	A	/A0286-TYR OH	A	/A0357-HIS ND1	2.5	SS	71	7.5		1402
1n3a.nb	A	/A0013-HIS NE2	A	/A0178-TYR OH	2.5	SS	-111.6			23
1n54.nb	A	/A0276-HIS ND1	A	/A0282-TYR OH	2.5	SS	6	9.9		1286
1nb7.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.5	SS	15	9.7		479
1nc3.nb	A	/A0097-TYR OH	A	/A0180-HIS ND1	2.5	SS	83	9.6		599
1nd6.nb	C	/C2237-HIS ND1	C	/C2247-TYR OH	2.5	SS	10	8.9		3940
1ndy.nb	A	/A0238-HIS ND1	A	/A0240-TYR OH	2.5	SS	2	5.5		1788
1ngs.nb	A	/A0042-HIS ND1	A	/A0297-TYR OH	2.5	SS	255	9.7		232
1nhu.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.5	SS	15	9.2		690
1nhu.nb	B	/B0103-TYR OH	B	/B0118-HIS ND1	2.5	SS	15	9.1		4003
1nhv.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.5	SS	15	9.2		500
1nhv.nb	B	/B0103-TYR OH	B	/B0118-HIS ND1	2.5	SS	15	9.2		2891
1nik.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.5	SS	8	9.9		10239
1nop.nb	B	/B0462-TYR OH	B	/B0474-HIS NE2	2.5	SS	1212.0			3494
1np3.nb	B	/B0024-TYR OH	B	/B0029-HIS ND1	2.5	SS	5	5.9		1766
1nqh.nb	A	/A0477-HIS ND1	A	/A0505-TYR OH	2.5	SS	28	7.2		1818
1ntk.nb	A	/A0152-TYR OH	A	/A0243-HIS ND1	2.5	SS	91	9.1		729
1ntm.nb	A	/A0154-HIS NE2	A	/A0314-TYR OH	2.5	SS	16011.6			751
1ntm.nb	C	/C0107-TYR OH	C	/C0308-HIS ND1	2.5	SS	201	9.3		4080
1nty.nb	A	/A1292-HIS NE2	A	/A1324-TYR OH	2.5	SS	3211.9			446
1ntz.nb	A	/A0152-TYR OH	A	/A0243-HIS ND1	2.5	SS	91	9.1		730
1ntz.nb	A	/A0154-HIS NE2	A	/A0314-TYR OH	2.5	SS	16011.6			745
1ntz.nb	A	/A0279-HIS ND1	A	/A0284-TYR OH	2.5	SS	5	9.7		1236
1ntz.nb	C	/C0107-TYR OH	C	/C0308-HIS ND1	2.5	SS	201	9.4		4100
1nu1.nb	A	/A0154-HIS NE2	A	/A0314-TYR OH	2.5	SS	16011.5			744
1nuh.nb	A	/A0343-TYR OH	A	/A0413-HIS NE2	2.5	SS	7010.9			1878
1nur.nb	B	/B0063-HIS ND1	B	/B0226-TYR OH	2.5	SS	-1	8.7		1684
1nus.nb	B	/B0063-HIS ND1	B	/B0226-TYR OH	2.5	SS	-1	8.7		1574
1nzy.nb	A	/A0150-TYR OH	A	/A0218-HIS ND1	2.5	SS	6810.3			946
1nzy.nb	B	/B0150-TYR OH	B	/B0218-HIS ND1	2.5	SS	6810.3			2639
1o1b.nb	A	/A0583-HIS NE2	A	/A0590-TYR OH	2.5	SS	712.0			2460
1o1b.nb	D	/D0583-HIS NE2	D	/D0590-TYR OH	2.5	SS	712.0			6699
1o1b.nb	G	/G0583-HIS NE2	G	/G0590-TYR OH	2.5	SS	712.0			10789
1o1b.nb	J	/J0583-HIS NE2	J	/J0590-TYR OH	2.5	SS	712.0			14882
1o1f.nb	A	/A0583-HIS NE2	A	/A0590-TYR OH	2.5	SS	712.0			2460
1o1f.nb	D	/D0583-HIS NE2	D	/D0590-TYR OH	2.5	SS	712.0			6697
1o1f.nb	G	/G0583-HIS NE2	G	/G0590-TYR OH	2.5	SS	712.0			10786
1o1f.nb	J	/J0583-HIS NE2	J	/J0590-TYR OH	2.5	SS	712.0			14878
1o3p.nb	B	/B0094-TYR OH	B	/B0099-HIS ND1	2.5	SS	7	7.0		656
1o5a.nb	B	/B0094-TYR OH	B	/B0099-HIS ND1	2.5	SS	7	7.0		638
1o5b.nb	B	/B0094-TYR OH	B	/B0099-HIS ND1	2.5	SS	7	7.0		642
1o67.nb	C	/C0069-HIS ND1	C	/C0156-TYR OH	2.5	SS	87	8.0		1965
1o88.nb	A	/A0228-HIS ND1	A	/A0320-TYR OH	2.5	SS	9210.8			1394
1o8e.nb	A	/A0228-HIS ND1	A	/A0320-TYR OH	2.5	SS	9211.0			1440
1o8g.nb	A	/A0228-HIS ND1	A	/A0320-TYR OH	2.5	SS	9210.9			1350
1o8j.nb	A	/A0228-HIS ND1	A	/A0320-TYR OH	2.5	SS	9211.0			1402
1o8k.nb	A	/A0228-HIS ND1	A	/A0320-TYR OH	2.5	SS	9211.0			1423
1o94.nb	B	/B0416-HIS ND1	B	/B0478-TYR OH	2.5	SS	62	9.8		5095
1o95.nb	B	/B0169-TYR OH	B	/B0172-HIS ND1	2.5	SS	3	8.7		3820
1o95.nb	B	/B0416-HIS ND1	B	/B0478-TYR OH	2.5	SS	62	9.9		4879
1ods.nb	B	/B0049-TYR OH	B	/B0100-HIS ND1	2.5	SS	51	9.3		1618

1oid.nb	A	/A0038-HIS	NE2	A	/A0312-TYR	OH	2.5	SS	27411.3	102
1ols.nb	A	/A0202-HIS	ND1	A	/A0246-TYR	OH	2.5	SS	44 8.9	1312
1olx.nb	A	/A0202-HIS	ND1	A	/A0246-TYR	OH	2.5	SS	44 8.9	1250
1ooc.nb	A	/A0251-HIS	ND1	A	/A0337-TYR	OH	2.5	SS	8611.2	1111
1ooc.nb	B	/B0251-HIS	ND1	B	/B0337-TYR	OH	2.5	SS	8611.2	2593
1oqz.nb	A	/A0393-HIS	NE2	A	/A0433-TYR	OH	2.5	SS	4011.6	1870
1oqz.nb	B	/B0393-HIS	NE2	B	/B0433-TYR	OH	2.5	SS	4011.6	4910
1or0.nb	D	/D0224-HIS	NE2	D	/D0264-TYR	OH	2.5	SS	4011.7	4300
1ord.nb	B	/B0192-TYR	OH	B	/B0382-HIS	ND1	2.5	SS	19010.1	3870
1orv.nb	A	/A0735-TYR	OH	A	/A0750-HIS	ND1	2.5	SS	15 9.4	2897
1orw.nb	C	/C0735-TYR	OH	C	/C0750-HIS	ND1	2.5	SS	15 9.4	8846
1osb.nb	A	/A0110-HIS	ND1	A	/A0196-TYR	OH	2.5	SS	86 8.5	585
1osg.nb	B	/B0201-TYR	OH	B	/B0210-HIS	ND1	2.5	SS	910.0	793
1ou5.nb	A	/A0172-TYR	OH	A	/A0186-HIS	ND1	2.5	SS	1410.8	593
1ou5.nb	B	/B0172-TYR	OH	B	/B0186-HIS	ND1	2.5	SS	1410.8	1896
1ozf.nb	B	/B0302-HIS	ND1	B	/B0314-TYR	OH	2.5	SS	12 9.4	4892
1ozg.nb	B	/B0302-HIS	ND1	B	/B0314-TYR	OH	2.5	SS	12 9.3	5108
1p1h.nb	A	/A0187-TYR	OH	A	/A0219-HIS	ND1	2.5	SS	3211.1	761
1p7p.nb	A	/A0028-HIS	ND1	A	/A0091-TYR	OH	2.5	SS	63 9.6	221
1p7t.nb	A	/A0394-HIS	NE2	A	/A0707-TYR	OH	2.5	SS	-112.7	1718
1p8d.nb	B	/B0270-HIS	NE2	B	/B0335-TYR	OH	2.5	SS	6511.6	1391
1pem.nb	A	/A0537-TYR	OH	A	/A0656-HIS	ND1	2.5	SS	119 9.9	2325
1peu.nb	A	/A0109-TYR	OH	A	/A0125-HIS	ND1	2.5	SS	16 7.9	468
1pfx.nb	C	/C0185-HIS	ND1	C	/C0225-TYR	OH	2.5	SS	41 7.1	708
1pk0.nb	A	/A0311-HIS	ND1	A	/A0492-TYR	OH	2.5	SS	18110.2	93
1plu.nb	A	/A0228-HIS	ND1	A	/A0320-TYR	OH	2.5	SS	9210.8	1016
1pmt.nb	A	/A0106-HIS	ND1	A	/A0157-TYR	OH	2.5	SS	51 9.0	501
1po6.nb	A	/A0124-TYR	OH	A	/A0168-HIS	ND1	2.5	SS	44 7.8	685
1pp9.nb	A	/A0279-HIS	ND1	A	/A0284-TYR	OH	2.5	SS	5 9.8	1239
1pp9.nb	N	/N0279-HIS	ND1	N	/N0284-TYR	OH	2.5	SS	5 9.8	9237
1ppj.nb	C	/C0107-TYR	OH	C	/C0308-HIS	ND1	2.5	SS	201 9.5	4072
1ppj.nb	P	/P0107-TYR	OH	P	/P0308-HIS	ND1	2.5	SS	201 9.5	11942
1pq6.nb	B	/B0270-HIS	NE2	B	/B0335-TYR	OH	2.5	SS	6512.0	1449
1pq6.nb	C	/C0270-HIS	NE2	C	/C0335-TYR	OH	2.5	SS	6511.6	2649
1pqc.nb	A	/A0270-HIS	NE2	A	/A0335-TYR	OH	2.5	SS	6511.3	237
1pth.nb	A	/A0234-TYR	OH	A	/A0309-HIS	ND1	2.5	SS	7510.0	944
1pth.nb	B	/B0234-TYR	OH	B	/B0309-HIS	ND1	2.5	SS	7510.0	3335
1pv6.nb	A	/A0236-TYR	OH	A	/A0322-HIS	ND1	2.5	SS	86 9.8	1045
1pv6.nb	B	/B0236-TYR	OH	B	/B0322-HIS	ND1	2.5	SS	86 9.8	2830
1pvq.nb	A	/A0074-TYR	OH	A	/A0091-HIS	ND1	2.5	SS	17 9.4	248
1pvr.nb	A	/A0074-TYR	OH	A	/A0091-HIS	ND1	2.5	SS	17 9.5	252
1pwx.nb	B	/B0177-TYR	OH	B	/B0201-HIS	NE2	2.5	SS	2410.6	2399
1pxx.nb	D	/D3234-TYR	OH	D	/D3309-HIS	ND1	2.5	SS	75 9.9	8029
1q22.nb	A	/A0144-TYR	OH	A	/A0192-HIS	ND1	2.5	SS	4810.7	643
1q32.nb	D	/D0305-HIS	ND1	D	/D0371-TYR	OH	2.5	SS	-1 7.6	5956
1qag.nb	A	/A0167-TYR	OH	A	/A0190-HIS	ND1	2.5	SS	23 9.6	573
1qb4.nb	A	/A0402-HIS	NE2	A	/A0472-TYR	OH	2.5	SS	7012.1	1916
1qc6.nb	B	/B2071-TYR	OH	B	/B2079-HIS	ND1	2.5	SS	8 7.3	676
1qe0.nb	A	/A0033-TYR	OH	A	/A0149-HIS	ND1	2.5	SS	-110.5	163
1qfg.nb	A	/A0599-TYR	OH	A	/A0623-HIS	ND1	2.5	SS	24 7.7	3030
1qfj.nb	A	/A0063-HIS	ND1	A	/A0146-TYR	OH	2.5	SS	-110.6	328
1qfk.nb	H	/H0241-HIS	ND1	H	/H0383-TYR	OH	2.5	SS	-1 9.1	839
1qji.nb	A	/A0141-TYR	OH	A	/A0148-HIS	NE2	2.5	SS	7 9.8	1034
1qlt.nb	A	/A0149-HIS	ND1	A	/A0408-TYR	OH	2.5	SS	25910.0	849
1qnl.nb	A	/A0108-TYR	OH	A	/A0335-HIS	NE2	2.5	SS	-111.1	488
1qvb.nb	B	/B0058-TYR	OH	B	/B0066-HIS	NE2	2.5	SS	8 9.6	3177

1qzr.nb	A	/A0020-HIS ND1	A	/A0028-TYR OH	2.5	SS	8	9.8	91
1r2b.nb	A	/A0046-HIS ND1	A	/A0091-TYR OH	2.5	SS	4510.1		218
1r5u.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.5	SS	8	9.9	10194
1r5x.nb	B	/B0019-HIS ND1	B	/B0098-TYR OH	2.5	SS	-1	9.6	632
1r9s.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.5	SS	8	9.9	10234
1rb8.nb	F	/F0109-TYR OH	F	/F0125-HIS ND1	2.5	SS	16	8.6	564
1rdy.nb	B	/B0279-TYR OH	B	/B0311-HIS ND1	2.5	SS	32	8.5	2665
1rdz.nb	B	/B0164-TYR OH	B	/B0253-HIS ND1	2.5	SS	89	9.0	2269
1rfu.nb	A	/A0079-TYR OH	A	/A0246-HIS ND1	2.5	SS	167	9.7	343
1rfu.nb	C	/C0079-TYR OH	C	/C0246-HIS ND1	2.5	SS	167	9.7	2862
1rfu.nb	D	/D0079-TYR OH	D	/D0246-HIS ND1	2.5	SS	167	9.7	4123
1rj2.nb	A	/A0693-HIS NE2	A	/A0725-TYR OH	2.5	SS	3211.7		360
1rj2.nb	D	/D0693-HIS NE2	D	/D0725-TYR OH	2.5	SS	3211.7		1667
1rj2.nb	J	/J0693-HIS NE2	J	/J0725-TYR OH	2.5	SS	3212.3		4309
1rj5.nb	B	/B0051-TYR OH	B	/B0122-HIS NE2	2.5	SS	6912.7		1452
1rj7.nb	D	/D0252-HIS ND1	D	/D0304-TYR OH	2.5	SS	52	9.1	1070
1rj7.nb	G	/G0252-HIS ND1	G	/G0304-TYR OH	2.5	SS	52	9.3	2654
1rj8.nb	G	/G0252-HIS ND1	G	/G0304-TYR OH	2.5	SS	52	9.2	3118
1rm6.nb	B	/B0046-HIS ND1	B	/B0141-TYR OH	2.5	SS	9510.6		3456
1rp7.nb	B	/B0213-HIS ND1	B	/B0538-TYR OH	2.5	SS	-1	8.9	4461
1rp9.nb	A	/A0310-TYR OH	A	/A0326-HIS ND1	2.5	SS	16	9.5	2255
1rpk.nb	A	/A0310-TYR OH	A	/A0326-HIS ND1	2.5	SS	16	9.5	2443
1rqr.nb	A	/A0211-HIS ND1	A	/A0284-TYR OH	2.5	SS	73	9.8	961
1ru7.nb	F	/F0522-TYR OH	F	/F0611-HIS ND1	2.5	SS	89	8.7	4875
1ru7.nb	H	/H0522-TYR OH	H	/H0611-HIS ND1	2.5	SS	89	8.7	6668
1ruy.nb	I	/I0642-HIS NE2	I	/I0657-TYR OH	2.5	SS	1512.5		1715
1ruy.nb	K	/K0642-HIS NE2	K	/K0657-TYR OH	2.5	SS	1512.5		3484
1ruy.nb	M	/M0642-HIS NE2	M	/M0657-TYR OH	2.5	SS	1512.5		5249
1rv0.nb	K	/K0642-HIS NE2	K	/K0657-TYR OH	2.5	SS	1512.7		3468
1rve.nb	B	/B0072-TYR OH	B	/B0131-HIS ND1	2.5	SS	5910.3		1187
1rvt.nb	K	/K0522-TYR OH	K	/K0611-HIS ND1	2.5	SS	89	8.7	3030
1rvt.nb	K	/K0642-HIS NE2	K	/K0657-TYR OH	2.5	SS	1512.6		3467
1rvt.nb	M	/M0522-TYR OH	M	/M0611-HIS ND1	2.5	SS	89	8.8	4801
1rvt.nb	M	/M0642-HIS NE2	M	/M0657-TYR OH	2.5	SS	1512.6		5242
1rvu.nb	A	/A0347-TYR OH	A	/A0426-HIS ND1	2.5	SS	79	9.1	1654
1rvx.nb	D	/D0522-TYR OH	D	/D0611-HIS ND1	2.5	SS	89	8.7	3104
1rvx.nb	J	/J0522-TYR OH	J	/J0611-HIS ND1	2.5	SS	89	8.8	8498
1rvy.nb	A	/A0347-TYR OH	A	/A0426-HIS ND1	2.5	SS	79	9.1	1626
1rvy.nb	B	/B0347-TYR OH	B	/B0426-HIS ND1	2.5	SS	79	9.0	3781
1rvz.nb	D	/D0522-TYR OH	D	/D0611-HIS ND1	2.5	SS	89	8.6	3088
1s0w.nb	C	/C1041-HIS NE2	C	/C1050-TYR OH	2.5	SS	912.6		1611
1s36.nb	A	/A0175-HIS NE2	A	/A0190-TYR OH	2.5	SS	1510.1		1136
1s4i.nb	B	/B0088-TYR OH	B	/B0166-HIS NE2	2.5	SS	7811.9		373
1s4i.nb	D	/D0088-TYR OH	D	/D0166-HIS NE2	2.5	SS	7811.9		2875
1s5g.nb	A	/A0582-HIS NE2	A	/A0589-TYR OH	2.5	SS	711.6		2398
1s76.nb	D	/D0486-HIS ND1	D	/D0518-TYR OH	2.5	SS	32	9.0	1925
1sb3.nb	E	/E0046-HIS ND1	E	/E0141-TYR OH	2.5	SS	9510.6		8611
1sqb.nb	B	/B0164-HIS NE2	B	/B0316-TYR OH	2.5	SS	15211.7		2602
1sqp.nb	A	/A0154-HIS NE2	A	/A0314-TYR OH	2.5	SS	16011.6		753
1srq.nb	A	/A0090-TYR OH	A	/A0099-HIS NE2	2.5	SS	910.2		63
1st0.nb	B	/B0217-TYR OH	B	/B0279-HIS ND1	2.5	SS	62	7.2	1067
1sxg.nb	A	/A0223-TYR OH	A	/A0256-HIS ND1	2.5	SS	33	9.6	738
1sxh.nb	A	/A0223-TYR OH	A	/A0256-HIS ND1	2.5	SS	33	9.4	711
1sxi.nb	N	/N0223-TYR OH	N	/N0256-HIS ND1	2.5	SS	-1	9.6	11347
1t0r.nb	A	/A0279-TYR OH	A	/A0329-HIS ND1	2.5	SS	50	9.2	1619
1t8r.nb	A	/A0209-TYR OH	A	/A0452-HIS ND1	2.5	SS	243	8.7	833

1t8s.nb	A	/A0209-TYR OH	A	/A0452-HIS ND1	2.5	SS	-1	8.9		795
1t8s.nb	C	/C0209-TYR OH	C	/C0452-HIS ND1	2.5	SS	-1	8.9		4428
1t8s.nb	D	/D0209-TYR OH	D	/D0452-HIS ND1	2.5	SS	-1	9.0		6221
1t8s.nb	E	/E0209-TYR OH	E	/E0452-HIS ND1	2.5	SS	-1	8.9		7979
1t8s.nb	F	/F0209-TYR OH	F	/F0452-HIS ND1	2.5	SS	-1	8.9		9750
1t8w.nb	A	/A0209-TYR OH	A	/A0452-HIS ND1	2.5	SS	243	8.8		828
1t8w.nb	C	/C0209-TYR OH	C	/C0452-HIS ND1	2.5	SS	-1	8.9		4618
1t8y.nb	A	/A0209-TYR OH	A	/A0452-HIS ND1	2.5	SS	243	8.9		831
1t8y.nb	C	/C0209-TYR OH	C	/C0452-HIS ND1	2.5	SS	-1	8.9		4630
1t8y.nb	D	/D0209-TYR OH	D	/D0452-HIS ND1	2.5	SS	-1	8.9		6502
1ti8.nb	A	/A0183-HIS ND1	A	/A0195-TYR OH	2.5	SS	12	10.4		891
1tkl.nb	A	/A0126-HIS ND1	A	/A0163-TYR OH	2.5	SS	37	8.6		684
1tlb.nb	S	/S0201-HIS ND1	S	/S0273-TYR OH	2.5	SS	72	10.3		4717
1tlb.nb	U	/U0126-HIS ND1	U	/U0163-TYR OH	2.5	SS	37	8.9		5621
1tls.nb	A	/A0147-HIS ND1	A	/A0181-TYR OH	2.5	SS	34	9.6		892
1tly.nb	A	/A0183-TYR OH	A	/A0218-HIS ND1	2.5	SS	35	7.5		624
1tly.nb	B	/B0183-TYR OH	B	/B0218-HIS ND1	2.5	SS	35	7.5		1570
1tw9.nb	E	/E0098-TYR OH	E	/E0163-HIS NE2	2.5	SS	-11	1.3		3697
1tyh.nb	A	/A0050-HIS ND1	A	/A0117-TYR OH	2.5	SS	67	8.5		321
1u1l.nb	A	/A0124-TYR OH	A	/A0168-HIS ND1	2.5	SS	44	7.8		643
1u1m.nb	A	/A0124-TYR OH	A	/A0168-HIS ND1	2.5	SS	44	7.7		624
1u1o.nb	A	/A0124-TYR OH	A	/A0168-HIS ND1	2.5	SS	44	7.8		594
1u1r.nb	A	/A0124-TYR OH	A	/A0168-HIS ND1	2.5	SS	44	7.9		786
1u67.nb	A	/A0234-TYR OH	A	/A0309-HIS ND1	2.5	SS	75	10.1		952
1u88.nb	B	/B0031-HIS ND1	B	/B0057-TYR OH	2.5	SS	26	9.7		979
1u8e.nb	B	/B0735-TYR OH	B	/B0750-HIS ND1	2.5	SS	15	9.4		5851
1ult.nb	A	/A0117-HIS ND1	A	/A0183-TYR OH	2.5	SS	66	9.8		721
1ulz.nb	A	/A0357-TYR OH	A	/A0369-HIS ND1	2.5	SS	12	11.8		2168
1upv.nb	A	/A0270-HIS NE2	A	/A0335-TYR OH	2.5	SS	65	11.4		228
1usw.nb	A	/A0025-TYR OH	A	/A0132-HIS ND1	2.5	SS	107	9.6		165
1uth.nb	B	/B0171-TYR OH	B	/B0206-HIS ND1	2.5	SS	35	9.4		1683
1uvh.nb	B	/B0095-TYR OH	B	/B0105-HIS ND1	2.5	SS	10	9.6		1090
1uvh.nb	C	/C0095-TYR OH	C	/C0105-HIS ND1	2.5	SS	10	9.6		1757
1uvr.nb	A	/A0197-HIS ND1	A	/A0333-TYR OH	2.5	SS	-11	0.0		688
1uyo.nb	X	/X1063-TYR OH	X	/X1074-HIS ND1	2.5	SS	11	7.4		878
1v26.nb	A	/A0117-HIS ND1	A	/A0183-TYR OH	2.5	SS	66	9.9		782
1v35.nb	A	/A0268-HIS ND1	A	/A0412-TYR OH	2.5	SS	-1	8.6		867
1v9k.nb	B	/B0242-HIS ND1	B	/B0261-TYR OH	2.5	SS	19	9.1		1960
1vb2.nb	A	/A0140-HIS ND1	A	/A0164-TYR OH	2.5	SS	24	7.1		378
1vch.nb	A	/A0068-HIS ND1	A	/A0078-TYR OH	2.5	SS	10	7.3		368
1vel.nb	F	/F0028-TYR OH	F	/F0141-HIS ND1	2.5	SS	113	10.4		3715
1vh2.nb	A	/A0066-TYR OH	A	/A0113-HIS ND1	2.5	SS	47	10.3		386
1vhk.nb	A	/A0004-TYR OH	A	/A0028-HIS ND1	2.5	SS	24	9.9		18
1vld.nb	O	/O0145-HIS NE2	O	/O0496-TYR OH	2.5	SS	351	10.0		5554
1vrw.nb	A	/A0268-HIS ND1	A	/A0412-TYR OH	2.5	SS	-1	8.6		755
1vsa.nb	B	/B0172-TYR OH	B	/B0186-HIS ND1	2.5	SS	14	5.4		1045
1w1i.nb	G	/G0238-HIS ND1	G	/G0240-TYR OH	2.5	SS	2	5.9	15	876
1w1l.nb	A	/A0149-HIS ND1	A	/A0408-TYR OH	2.5	SS	259	10.1		668
1w1z.nb	B	/B0134-HIS ND1	B	/B0225-TYR OH	2.5	SS	91	10.5		2385
1w2c.nb	A	/A0289-TYR OH	A	/A0305-HIS ND1	2.5	SS	16	8.0		562
1w37.nb	D	/D0026-HIS ND1	D	/D0255-TYR OH	2.5	SS	229	8.0		5001
1w3t.nb	B	/B0026-HIS ND1	B	/B0255-TYR OH	2.5	SS	229	8.0		2028
1w5s.nb	A	/A0309-HIS ND1	A	/A0337-TYR OH	2.5	SS	28	8.4		1488
1w5s.nb	B	/B0113-TYR OH	B	/B0138-HIS ND1	2.5	SS	25	11.0		2459
1w5t.nb	A	/A0309-HIS ND1	A	/A0337-TYR OH	2.5	SS	28	9.1		1449
1w5t.nb	B	/B0309-HIS ND1	B	/B0337-TYR OH	2.5	SS	28	9.0		3268

1w87.nb	A	/A0042-HIS ND1	A	/A0201-TYR OH	2.5	SS	159	9.8	178
1w87.nb	B	/B0042-HIS ND1	B	/B0201-TYR OH	2.5	SS	159	9.6	1447
1w8k.nb	A	/A0147-TYR OH	A	/A0165-HIS ND1	2.5	SS	18	9.1	632
1w93.nb	A	/A0021-TYR OH	A	/A0413-HIS NE2	2.5	SS	39212.1		34
1waf.nb	A	/A0138-HIS ND1	A	/A0201-TYR OH	2.5	SS	63	9.6	587
1waf.nb	B	/B0138-HIS ND1	B	/B0201-TYR OH	2.5	SS	63	9.6	4169
1waj.nb	A	/A0138-HIS ND1	A	/A0201-TYR OH	2.5	SS	63	9.5	654
1wcm.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.6		1636
1wcm.nb	A	/A0804-TYR OH	A	/A0816-HIS NE2	2.5	SS	1211.5		2922
1wmr.nb	A	/A0231-HIS ND1	A	/A0285-TYR OH	2.5	SS	54	9.2	1262
1wmr.nb	B	/B0231-HIS ND1	B	/B0285-TYR OH	2.5	SS	54	9.5	4462
1wuu.nb	A	/A0044-HIS ND1	A	/A0047-TYR OH	2.5	SS	3	6.7	242
1wuu.nb	B	/B0044-HIS ND1	B	/B0047-TYR OH	2.5	SS	3	7.0	1842
1wyu.nb	F	/F0237-TYR OH	F	/F0261-HIS ND1	2.5	SS	24	8.4	10083
1wyv.nb	B	/B0237-TYR OH	B	/B0261-HIS ND1	2.5	SS	24	8.4	2764
1x1u.nb	E	/E0017-HIS ND1	E	/E0030-TYR OH	2.5	SS	13	8.9	2529
1x24.nb	A	/A0053-TYR OH	A	/A0103-HIS NE2	2.5	SS	5012.5		216
1x33.nb	A	/A0140-HIS ND1	A	/A0164-TYR OH	2.5	SS	24	7.1	341
1x35.nb	A	/A0140-HIS ND1	A	/A0164-TYR OH	2.5	SS	24	7.2	344
1x35.nb	B	/B0140-HIS ND1	B	/B0164-TYR OH	2.5	SS	24	7.1	1047
1x35.nb	C	/C0140-HIS ND1	C	/C0164-TYR OH	2.5	SS	24	7.1	1815
1x6v.nb	B	/B0575-TYR OH	B	/B0580-HIS ND1	2.5	SS	5	7.5	3670
1x8e.nb	B	/B0099-TYR OH	B	/B0136-HIS NE2	2.5	SS	3711.1		1074
1xa9.nb	A	/A0075-TYR OH	A	/A0198-HIS NE2	2.5	SS	12310.4		435
1xd4.nb	A	/A0349-HIS NE2	A	/A0353-TYR OH	2.5	SS	4	6.7	714
1xd4.nb	B	/B0349-HIS NE2	B	/B0353-TYR OH	2.5	SS	4	6.7	4105
1xdv.nb	A	/A0349-HIS NE2	A	/A0353-TYR OH	2.5	SS	4	6.7	705
1xdv.nb	B	/B0349-HIS NE2	B	/B0353-TYR OH	2.5	SS	4	6.7	3869
1xkv.nb	B	/B0027-HIS ND1	B	/B0100-TYR OH	2.5	SS	7310.6		3425
1xns.nb	A	/A0074-TYR OH	A	/A0091-HIS ND1	2.5	SS	17	9.6	270
1xr2.nb	A	/A0233-TYR OH	A	/A0313-HIS NE2	2.5	SS	8011.5		1079
1xsi.nb	B	/B0487-TYR OH	B	/B0522-HIS ND1	2.5	SS	35	9.9	5514
1xvb.nb	A	/A0292-TYR OH	A	/A0344-HIS ND1	2.5	SS	52	8.8	1332
1xxm.nb	C	/C1041-HIS NE2	C	/C1050-TYR OH	2.5	SS	912.6		1716
1y1v.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.5	SS	21	8.9	13576
1y77.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.6		1647
1y77.nb	A	/A0804-TYR OH	A	/A0816-HIS NE2	2.5	SS	1211.5		2933
1y7h.nb	D	/D0015-HIS NE2	D	/D0161-TYR OH	2.5	SS	14612.8		3318
1ydd.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.7		645
1ygz.nb	B	/B0116-HIS ND1	B	/B0118-TYR OH	2.5	SS	2	5.3	1248
1ygz.nb	D	/D0116-HIS ND1	D	/D0118-TYR OH	2.5	SS	2	5.4	2729
1yi7.nb	B	/B0025-TYR OH	B	/B0256-HIS ND1	2.5	SS	23110.0		2371
1yoz.nb	A	/A0078-TYR OH	A	/A0086-HIS ND1	2.5	SS	8	9.7	455
1yp3.nb	D	/D0071-TYR OH	D	/D0134-HIS NE2	2.5	SS	-111.6		5531
1yqx.nb	A	/A0104-HIS NE2	A	/A0148-TYR OH	2.5	SS	4412.0		533
1yr8.nb	A	/A0142-TYR OH	A	/A0178-HIS ND1	2.5	SS	36	8.5	695
1yra.nb	B	/B0142-TYR OH	B	/B0178-HIS ND1	2.5	SS	36	8.3	2241
1yym.nb	G	/G0249-HIS ND1	G	/G0486-TYR OH	2.5	SS	-110.1		378
1yym.nb	P	/P1249-HIS ND1	P	/P1486-TYR OH	2.5	SS	-110.0		3092
1z68.nb	B	/B0338-HIS ND1	B	/B0364-TYR OH	2.5	SS	2611.6		4192
1z9y.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.5		779
1zeb.nb	A	/A0319-HIS ND1	A	/A0393-TYR OH	2.5	SS	74	8.5	2639
1zeb.nb	A	/A0460-HIS ND1	A	/A0471-TYR OH	2.5	SS	11	8.6	3607
1zel.nb	B	/B0084-TYR OH	B	/B0109-HIS NE2	2.5	SS	2512.8		2196
1zfj.nb	A	/A0477-HIS ND1	A	/A0490-TYR OH	2.5	SS	13	9.5	2802
1zgf.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.5		735

1zgl.nb	E	/E0028-HIS ND1	E	/E0047-TYR OH	2.5	SS	19	8.6	3188
1zi7.nb	B	/B0164-TYR OH	B	/B0418-HIS ND1	2.5	SS	251	7.9	2536
1zk8.nb	A	/A0102-TYR OH	A	/A0149-HIS ND1	2.5	SS	47	9.9	600
1zm2.nb	B	/B0426-HIS ND1	B	/B0502-TYR OH	2.5	SS	76	9.3	3476
1zm2.nb	D	/D0426-HIS ND1	D	/D0502-TYR OH	2.5	SS	76	9.2	7538
1zm2.nb	F	/F0426-HIS ND1	F	/F0502-TYR OH	2.5	SS	76	9.3	11610
1zw6.nb	A	/A0094-HIS ND1	A	/A0137-TYR OH	2.5	SS	43	9.7	665
1zx0.nb	D	/D0134-TYR OH	D	/D0147-HIS ND1	2.5	SS	1310.5		5313
1zxb.nb	B	/B0268-HIS ND1	B	/B0412-TYR OH	2.5	SS	-1	8.3	2010
1zyl.nb	A	/A0133-HIS ND1	A	/A0252-TYR OH	2.5	SS	119	9.3	558
2a06.nb	A	/A0154-HIS NE2	A	/A0314-TYR OH	2.5	SS	-111.5		758
2a06.nb	N	/N0154-HIS NE2	N	/N0314-TYR OH	2.5	SS	-111.5		8704
2a06.nb	N	/N0279-HIS ND1	N	/N0284-TYR OH	2.5	SS	5	9.7	9205
2a0f.nb	A	/A0170-HIS ND1	A	/A0197-TYR OH	2.5	SS	27	8.7	899
2a3v.nb	A	/A0130-TYR OH	A	/A0276-HIS ND1	2.5	SS	146	9.7	549
2a3v.nb	C	/C0130-TYR OH	C	/C0276-HIS ND1	2.5	SS	146	9.7	3024
2a6w.nb	A	/A0167-TYR OH	A	/A0173-HIS ND1	2.5	SS	6	6.5	1010
2a89.nb	A	/A0055-TYR OH	A	/A0345-HIS ND1	2.5	SS	29010.5		449
2aa4.nb	A	/A0215-HIS ND1	A	/A0256-TYR OH	2.5	SS	41	9.2	1146
2aaz.nb	F	/F0188-HIS ND1	F	/F0231-TYR OH	2.5	SS	43	9.5	7104
2aaz.nb	G	/G0188-HIS ND1	G	/G0231-TYR OH	2.5	SS	43	9.5	8367
2aaz.nb	H	/H0188-HIS ND1	H	/H0231-TYR OH	2.5	SS	43	9.5	9619
2acl.nb	F	/F0254-HIS NE2	F	/F0319-TYR OH	2.5	SS	6511.6		4881
2ae3.nb	B	/B0224-HIS NE2	B	/B0264-TYR OH	2.5	SS	4011.7		1963
2ae4.nb	B	/B0224-HIS NE2	B	/B0264-TYR OH	2.5	SS	4011.7		2076
2ah8.nb	A	/A0074-TYR OH	A	/A0199-HIS NE2	2.5	SS	12510.9		444
2aj8.nb	A	/A0735-TYR OH	A	/A0750-HIS ND1	2.5	SS	15	9.4	2914
2ajl.nb	I	/I0735-TYR OH	I	/I0750-HIS ND1	2.5	SS	15	9.5	2833
2av9.nb	L	/L0098-TYR OH	L	/L0118-HIS ND1	2.5	SS	20	8.1	6166
2avu.nb	E	/E0072-HIS ND1	E	/E0102-TYR OH	2.5	SS	30	7.8	1640
2az5.nb	D	/D0015-HIS ND1	D	/D0059-TYR OH	2.5	SS	44	9.1	1863
2b08.nb	A	/A0245-HIS ND1	A	/A0303-TYR OH	2.5	SS	5810.9		1670
2b2t.nb	A	/A0139-HIS ND1	A	/A0182-TYR OH	2.5	SS	43	9.4	738
2b2u.nb	A	/A0139-HIS ND1	A	/A0182-TYR OH	2.5	SS	43	9.4	492
2b2v.nb	A	/A0139-HIS ND1	A	/A0182-TYR OH	2.5	SS	43	9.4	593
2b2w.nb	A	/A0139-HIS ND1	A	/A0182-TYR OH	2.5	SS	43	9.4	733
2b2y.nb	A	/A0139-HIS ND1	A	/A0182-TYR OH	2.5	SS	43	9.4	705
2b63.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.8		1623
2b8k.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.6		1636
2b8q.nb	A	/A0053-HIS ND1	A	/A0058-TYR OH	2.5	SS	5	8.4	323
2bbc.nb	A	/A0330-TYR OH	A	/A0332-HIS ND1	2.5	SS	2	6.9	1776
2bbj.nb	B	/B0115-TYR OH	B	/B0120-HIS ND1	2.5	SS	5	7.9	1700
2bcc.nb	B	/B0164-HIS NE2	B	/B0316-TYR OH	2.5	SS	13611.7		2460
2bcj.nb	A	/A0562-HIS ND1	A	/A0580-TYR OH	2.5	SS	18	7.2	2199
2bhd.nb	A	/A0350-HIS NE2	A	/A0387-TYR OH	2.5	SS	3710.5		1820
2bhy.nb	A	/A0101-HIS ND1	A	/A0224-TYR OH	2.5	SS	123	9.1	758
2bjh.nb	A	/A0025-TYR OH	A	/A0132-HIS ND1	2.5	SS	107	9.6	179
2bjh.nb	C	/C0025-TYR OH	C	/C0132-HIS ND1	2.5	SS	107	9.3	2976
2bpb.nb	A	/A0057-HIS NE2	A	/A0236-TYR OH	2.5	SS	17912.4		394
2bpo.nb	B	/B0289-HIS ND1	B	/B0588-TYR OH	2.5	SS	-1	9.6	3711
2brl.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.5	SS	15	9.4	576
2bwe.nb	T	/T0046-TYR OH	T	/T0066-HIS ND1	2.5	SS	20	9.1	3870
2bwn.nb	B	/B0056-TYR OH	B	/B0217-HIS ND1	2.5	SS	161	9.3	1934
2bwo.nb	D	/D0222-TYR OH	D	/D0331-HIS ND1	2.5	SS	10910.0		4429
2bxy.nb	A	/A0101-HIS ND1	A	/A0224-TYR OH	2.5	SS	123	9.1	738
2c11.nb	A	/A0201-TYR OH	A	/A0203-HIS ND1	2.5	SS	2	6.1	667

2c1c.nb	A	/A0184-HIS NE2	A	/A0257-TYR OH	2.5	SS	7810.9	1151
2c4p.nb	B	/B0045-TYR OH	B	/B0075-HIS ND1	2.5	SS	30 9.7	891
2c5b.nb	C	/C0211-HIS ND1	C	/C0284-TYR OH	2.5	SS	7310.0	3655
2c8n.nb	A	/A0141-TYR OH	A	/A0157-HIS ND1	2.5	SS	1610.3	723
2c8n.nb	B	/B0141-TYR OH	B	/B0157-HIS ND1	2.5	SS	1610.3	2852
2c8n.nb	C	/C0141-TYR OH	C	/C0157-HIS ND1	2.5	SS	1610.4	5002
2c9k.nb	A	/A0579-HIS NE2	A	/A0586-TYR OH	2.5	SS	711.5	2667
2ca2.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.5	SS	7111.9	306
2ca3.nb	A	/A0057-HIS NE2	A	/A0236-TYR OH	2.5	SS	17912.3	386
2cbj.nb	B	/B0307-HIS ND1	B	/B0349-TYR OH	2.5	SS	4210.1	4383
2cbx.nb	A	/A0211-HIS ND1	A	/A0284-TYR OH	2.5	SS	73 9.6	1274
2cbx.nb	B	/B0211-HIS ND1	B	/B0284-TYR OH	2.5	SS	73 9.5	2945
2cc2.nb	A	/A0211-HIS ND1	A	/A0284-TYR OH	2.5	SS	73 9.7	1074
2cjp.nb	A	/A0268-TYR OH	A	/A0278-HIS NE2	2.5	SS	1011.1	1627
2cjr.nb	E	/E0299-TYR OH	E	/E0357-HIS NE2	2.5	SS	5812.1	2692
2cko.nb	A	/A0236-HIS ND1	A	/A0382-TYR OH	2.5	SS	14610.1	631
2cl6.nb	X	/X0094-HIS ND1	X	/X0137-TYR OH	2.5	SS	43 9.7	836
2cm3.nb	A	/A0124-TYR OH	A	/A0214-HIS NE2	2.5	SS	9012.1	870
2cmg.nb	B	/B0237-TYR OH	B	/B0242-HIS ND1	2.5	SS	5 7.2	2494
2cmh.nb	A	/A0237-TYR OH	A	/A0242-HIS ND1	2.5	SS	5 6.9	1168
2cn4.nb	B	/B0075-TYR OH	B	/B0083-HIS ND1	2.5	SS	8 6.5	1058
2cnb.nb	A	/A0200-TYR OH	A	/A0280-HIS NE2	2.5	SS	-110.9	857
2cnb.nb	C	/C0200-TYR OH	C	/C0280-HIS NE2	2.5	SS	-110.9	3875
2cnc.nb	A	/A0133-TYR OH	A	/A0178-HIS ND1	2.5	SS	45 8.4	803
2col.nb	A	/A0046-HIS ND1	A	/A0122-TYR OH	2.5	SS	76 8.8	247
2csx.nb	A	/A0237-TYR OH	A	/A0264-HIS NE2	2.5	SS	2711.3	959
2d3u.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.5	SS	15 9.2	696
2d74.nb	B	/B0062-HIS ND1	B	/B0100-TYR OH	2.5	SS	3810.0	2052
2df7.nb	A	/A0071-HIS NE2	A	/A0354-TYR OH	2.5	SS	28311.2	332
2df7.nb	H	/H0071-HIS NE2	H	/H0354-TYR OH	2.5	SS	-111.2	11115
2dl2.nb	A	/A0050-HIS NE2	A	/A0088-TYR OH	2.5	SS	3811.6	230
2du4.nb	A	/A0078-HIS ND1	A	/A0317-TYR OH	2.5	SS	-1 9.6	340
2dw7.nb	D	/D0106-HIS ND1	D	/D0297-TYR OH	2.5	SS	191 8.8	5419
2e6k.nb	B	/B0051-HIS ND1	B	/B0084-TYR OH	2.5	SS	3310.4	3102
2efb.nb	A	/A0193-TYR OH	A	/A0273-HIS ND1	2.5	SS	80 9.8	952
2ein.nb	A	/A0261-TYR OH	A	/A0395-HIS ND1	2.5	SS	134 9.9	1293
2eq7.nb	A	/A0002-TYR OH	A	/A0107-HIS NE2	2.5	SS	10512.4	12
2eu3.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.7	774
2exe.nb	A	/A0368-TYR OH	A	/A0442-HIS ND1	2.5	SS	74 9.8	810
2exj.nb	A	/A0363-HIS NE2	A	/A0460-TYR OH	2.5	SS	9712.2	1510
2exk.nb	B	/B0013-HIS NE2	B	/B0041-TYR OH	2.5	SS	2810.5	2283
2ez7.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.4	707
2f2h.nb	E	/E0487-TYR OH	E	/E0522-HIS ND1	2.5	SS	35 9.7	15373
2f4i.nb	C	/C0079-HIS ND1	C	/C0094-TYR OH	2.5	SS	-1 8.2	2363
2f4n.nb	C	/C0177-HIS ND1	C	/C0257-TYR OH	2.5	SS	-1 6.2	2528
2f55.nb	B	/B0350-TYR OH	B	/B0369-HIS ND1	2.5	SS	1910.7	2257
2f61.nb	A	/A0490-HIS ND1	A	/A0492-TYR OH	2.5	SS	2 6.5	2717
2fdc.nb	B	/B0034-HIS ND1	B	/B0391-TYR OH	2.5	SS	357 7.7	2289
2fgj.nb	C	/C0585-HIS ND1	C	/C0595-TYR OH	2.5	SS	10 8.9	2759
2fie.nb	L	/L0279-TYR OH	L	/L0311-HIS ND1	2.5	SS	32 8.3	5183
2fix.nb	L	/L0164-TYR OH	L	/L0253-HIS ND1	2.5	SS	89 9.0	4211
2flz.nb	B	/B0003-TYR OH	B	/B0028-HIS ND1	2.5	SS	2510.1	617
2fnj.nb	A	/A0102-HIS ND1	A	/A0230-TYR OH	2.5	SS	128 8.2	475
2fnq.nb	A	/A0581-HIS ND1	A	/A0584-TYR OH	2.5	SS	3 6.2	870
2fnq.nb	B	/B0581-HIS ND1	B	/B0584-TYR OH	2.5	SS	3 6.2	3737
2fw4.nb	B	/B0051-TYR OH	B	/B0122-HIS NE2	2.5	SS	7111.1	1870

2fwr.nb	A	/A0347-HIS NE2	A	/A0448-TYR OH	2.5	SS	10111.5		1344
2fym.nb	A	/A0274-HIS NE2	A	/A0302-TYR OH	2.5	SS	2810.3		1283
2fym.nb	C	/C0274-HIS NE2	C	/C0302-TYR OH	2.5	SS	2810.3		3198
2fym.nb	F	/F0274-HIS NE2	F	/F0302-TYR OH	2.5	SS	2810.3		7039
2fyu.nb	C	/C0107-TYR OH	C	/C0308-HIS ND1	2.5	SS	201	9.4	4180
2fzg.nb	C	/C0156-HIS ND1	C	/C0185-TYR OH	2.5	SS	29	7.8	3410
2g01.nb	A	/A0125-HIS ND1	A	/A0320-TYR OH	2.5	SS	195	8.8	476
2g39.nb	A	/A0463-TYR OH	A	/A0476-HIS ND1	2.5	SS	13	7.9	3134
2g39.nb	B	/B0463-TYR OH	B	/B0476-HIS ND1	2.5	SS	13	7.8	6339
2g4o.nb	C	/C0207-TYR OH	C	/C0209-HIS ND1	2.5	SS	2	7.0	3704
2g9z.nb	B	/B0109-TYR OH	B	/B0153-HIS ND1	2.5	SS	44	9.7	2444
2gge.nb	A	/A0035-TYR OH	A	/A0059-HIS ND1	2.5	SS	24	8.3	171
2gk4.nb	A	/A0041-TYR OH	A	/A0228-HIS NE2	2.5	SS	-112.1		322
2gmj.nb	A	/A0216-HIS ND1	A	/A0238-TYR OH	2.5	SS	22	8.9	1006
2guw.nb	A	/A0209-TYR OH	A	/A0452-HIS ND1	2.5	SS	-1	8.9	656
2gv9.nb	B	/B0065-HIS ND1	B	/B0067-TYR OH	2.5	SS	2	5.8	3959
2gv9.nb	B	/B0851-TYR OH	B	/B0912-HIS NE2	2.5	SS	6110.7		6923
2gxa.nb	B	/B0482-HIS ND1	B	/B0532-TYR OH	2.5	SS	50	9.6	1879
2gxa.nb	L	/L0482-HIS ND1	L	/L0532-TYR OH	2.5	SS	5010.9		12586
2gz2.nb	B	/B0003-TYR OH	B	/B0342-HIS ND1	2.5	SS	339	9.7	2056
2h1e.nb	A	/A0021-HIS ND1	A	/A0081-TYR OH	2.5	SS	60	9.0	82
2h7v.nb	C	/C0505-TYR OH	C	/C0568-HIS ND1	2.5	SS	-1	7.9	1798
2hd6.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.6		801
2hd9.nb	A	/A0081-HIS ND1	A	/A0088-TYR OH	2.5	SS	710.1		652
2hh9.nb	B	/B0109-TYR OH	B	/B0153-HIS ND1	2.5	SS	44	9.6	2595
2hih.nb	B	/B0071-HIS ND1	B	/B0136-TYR OH	2.5	SS	65	9.3	2086
2ho5.nb	A	/A0014-HIS ND1	A	/A0046-TYR OH	2.5	SS	3210.4		85
2hoc.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.5	SS	7111.7		325
2hsg.nb	A	/A0223-TYR OH	A	/A0256-HIS ND1	2.5	SS	33	9.4	929
2ht8.nb	A	/A0113-HIS ND1	A	/A0069ATYR OH	2.5	SS	57	8.1	215
2htu.nb	A	/A0113-HIS ND1	A	/A0070-TYR OH	2.5	SS	57	8.3	175
2hwv.nb	A	/A0167-TYR OH	A	/A0180-HIS NE2	2.5	SS	1311.0		202
2hyd.nb	A	/A0103-HIS ND1	A	/A0322-TYR OH	2.5	SS	219	8.8	470
2hyd.nb	A	/A0457-HIS ND1	A	/A0467-TYR OH	2.5	SS	10	8.2	2049
2hyd.nb	B	/B0103-HIS ND1	B	/B0322-TYR OH	2.5	SS	219	8.8	2945
2hyd.nb	B	/B0457-HIS ND1	B	/B0467-TYR OH	2.5	SS	10	8.2	4529
2i15.nb	C	/C0494-TYR OH	C	/C0516-HIS ND1	2.5	SS	22	9.6	1363
2i1r.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.5	SS	15	9.1	599
2i1w.nb	A	/A0109-TYR OH	A	/A0228-HIS ND1	2.5	SS	-1	8.7	617
2i1w.nb	D	/D0109-TYR OH	D	/D0228-HIS ND1	2.5	SS	-1	8.6	4437
2i2c.nb	A	/A0109-TYR OH	A	/A0228-HIS ND1	2.5	SS	119	8.6	661
2i4h.nb	A	/A1815-TYR OH	A	/A1903-HIS NE2	2.5	SS	-112.3		915
2i4o.nb	B	/B0174-TYR OH	B	/B0208-HIS ND1	2.5	SS	3410.1		2641
2i5y.nb	G	/G0249-HIS ND1	G	/G0486-TYR OH	2.5	SS	-110.1		370
2i6f.nb	C	/C0092-HIS ND1	C	/C0102-TYR OH	2.5	SS	10	9.6	2006
2i80.nb	A	/A0017-HIS NE2	A	/A0042-TYR OH	2.5	SS	2510.0		106
2i82.nb	A	/A0162-HIS ND1	A	/A0181-TYR OH	2.5	SS	19	9.8	843
2i87.nb	A	/A0017-HIS NE2	A	/A0042-TYR OH	2.5	SS	25	9.7	100
2i87.nb	B	/B0017-HIS NE2	B	/B0042-TYR OH	2.5	SS	2510.0		1670
2iag.nb	A	/A0177-TYR OH	A	/A0199-HIS NE2	2.5	SS	2210.3		923
2idg.nb	C	/C0068-TYR OH	C	/C0131-HIS ND1	2.5	SS	-110.1		1840
2ihc.nb	D	/D0048-HIS ND1	D	/D0092-TYR OH	2.5	SS	-110.0		1514
2iiv.nb	A	/A0735-TYR OH	A	/A0750-HIS ND1	2.5	SS	15	9.3	2880
2inn.nb	A	/A0282-TYR OH	A	/A0333-HIS ND1	2.5	SS	51	8.2	1340
2io9.nb	A	/A0271-HIS ND1	A	/A0331-TYR OH	2.5	SS	60	8.4	1267
2iok.nb	B	/B1373-HIS ND1	B	/B1537-TYR OH	2.5	SS	-1	9.6	1331

2ioq.nb	B	/B0246-TYR OH	B	/B0265-HIS ND1	2.5	SS	19	9.6	3008
2ist.nb	A	/A0234-HIS ND1	A	/A0253-TYR OH	2.5	SS	19	9.9	1420
2ixe.nb	A	/A0703-HIS ND1	A	/A0713-TYR OH	2.5	SS	10	8.5	1393
2izt.nb	A	/A0154-HIS ND1	A	/A0301-TYR OH	2.5	SS	14710.5		783
2j25.nb	B	/B0490-HIS ND1	B	/B0492-TYR OH	2.5	SS	2	6.3	4554
2j4y.nb	A	/A0206-TYR OH	A	/A0211-HIS NE2	2.5	SS	5	7.9	939
2j4y.nb	B	/B0206-TYR OH	B	/B0211-HIS NE2	2.5	SS	5	7.8	2312
2j62.nb	B	/B0307-HIS ND1	B	/B0349-TYR OH	2.5	SS	4210.2		4610
2ja5.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.6		1688
2ja5.nb	A	/A0804-TYR OH	A	/A0816-HIS NE2	2.5	SS	1211.3		2994
2ja7.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.5	SS	21	9.0	13801
2ja8.nb	K	/K0040-HIS ND1	K	/K0061-TYR OH	2.5	SS	21	8.9	13829
2jes.nb	O	/O0089-HIS ND1	O	/O0260-TYR OH	2.5	SS	-1	8.7	9998
2jes.nb	Q	/Q0089-HIS ND1	Q	/Q0260-TYR OH	2.5	SS	-1	8.6	11387
2jes.nb	S	/S0089-HIS ND1	S	/S0260-TYR OH	2.5	SS	-1	8.6	12774
2jh8.nb	A	/A0194-HIS ND1	A	/A0223-TYR OH	2.5	SS	29	7.3	880
2jj9.nb	A	/A0572-HIS NE2	A	/A0579-TYR OH	2.5	SS	712.1		3729
2jjk.nb	A	/A0279-TYR OH	A	/A0311-HIS ND1	2.5	SS	32	8.5	1561
2jjk.nb	D	/D0164-TYR OH	D	/D0253-HIS ND1	2.5	SS	89	8.9	5064
2jlb.nb	B	/B0326-TYR OH	B	/B0563-HIS NE2	2.5	SS	23712.5		4210
2mys.nb	A	/A0583-HIS NE2	A	/A0590-TYR OH	2.5	SS	712.0		2382
2nlk.nb	A	/A1210-TYR OH	A	/A1241-HIS NE2	2.5	SS	3110.8		1939
2nlk.nb	A	/A1262-TYR OH	A	/A1313-HIS NE2	2.5	SS	5111.3		2203
2npe.nb	A	/A0064-TYR OH	A	/A0100-HIS ND1	2.5	SS	36	9.4	396
2nvw.nb	B	/B0036-HIS ND1	B	/B0385-TYR OH	2.5	SS	-1	9.3	2385
2nvy.nb	A	/A0804-TYR OH	A	/A0816-HIS NE2	2.5	SS	1210.8		3266
2nvy.nb	C	/C0180-TYR OH	C	/C0188-HIS ND1	2.5	SS	8	9.7	11027
2nzw.nb	C	/C0130-HIS ND1	C	/C0151-TYR OH	2.5	SS	21	8.9	5556
2o0o.nb	A	/A0098-HIS ND1	A	/A0150-TYR OH	2.5	SS	52	9.1	37
2o1w.nb	B	/B0355-TYR OH	B	/B0374-HIS ND1	2.5	SS	19	8.8	2605
2o1w.nb	D	/D0355-TYR OH	D	/D0374-HIS ND1	2.5	SS	19	8.8	5889
2o2c.nb	A	/A0107-HIS ND1	A	/A0380-TYR OH	2.5	SS	273	8.9	302
2o2d.nb	A	/A0107-HIS ND1	A	/A0380-TYR OH	2.5	SS	273	8.8	327
2o2d.nb	B	/B0107-HIS ND1	B	/B0380-TYR OH	2.5	SS	273	8.8	2836
2o9i.nb	B	/B1242-HIS NE2	B	/B1306-TYR OH	2.5	SS	6411.4		1772
2ohk.nb	A	/A0181-HIS ND1	A	/A0184-TYR OH	2.5	SS	3	5.6	1069
2ojy.nb	A	/A0091-TYR OH	A	/A0428-HIS ND1	2.5	SS	337	7.3	1547
2ol4.nb	A	/A0268-HIS ND1	A	/A0412-TYR OH	2.5	SS	-1	8.6	861
2oos.nb	A	/A0268-HIS ND1	A	/A0412-TYR OH	2.5	SS	-1	8.6	929
2op1.nb	A	/A0268-HIS ND1	A	/A0412-TYR OH	2.5	SS	-1	8.6	861
2op5.nb	C	/C0039-TYR OH	C	/C0050-HIS ND1	2.5	SS	11	9.0	1193
2op5.nb	D	/D0039-TYR OH	D	/D0050-HIS ND1	2.5	SS	11	9.3	1651
2oq7.nb	B	/B0299-TYR OH	B	/B0343-HIS ND1	2.5	SS	44	9.8	3434
2oqv.nb	A	/A0735-TYR OH	A	/A0750-HIS ND1	2.5	SS	15	9.4	2807
2oqv.nb	B	/B0735-TYR OH	B	/B0750-HIS ND1	2.5	SS	15	9.3	5717
2otp.nb	A	/A0036-HIS NE2	A	/A0085-TYR OH	2.5	SS	-1	8.1	170
2oww.nb	A	/A0379-HIS ND1	A	/A0417-TYR OH	2.5	SS	3810.3		2412
2p0i.nb	F	/F0095-HIS ND1	F	/F0122-TYR OH	2.5	SS	-111.5		8498
2p0i.nb	G	/G0095-HIS ND1	G	/G0122-TYR OH	2.5	SS	-111.5		10085
2p1i.nb	G	/G0144-TYR OH	G	/G0213-HIS NE2	2.5	SS	-111.6		6974
2p2j.nb	A	/A0560-TYR OH	A	/A0597-HIS ND1	2.5	SS	37	7.4	2538
2p4s.nb	A	/A0220-HIS ND1	A	/A0251-TYR OH	2.5	SS	31	9.0	803
2p6x.nb	A	/A0142-TYR OH	A	/A0226-HIS NE2	2.5	SS	8412.2		996
2p90.nb	A	/A0147-HIS ND1	A	/A0204-TYR OH	2.5	SS	57	9.1	852
2pbh.nb	A	/A0037PTYR OH	A	/A0110-HIS ND1	2.5	SS	-1	9.4	148
2pec.nb	A	/A0228-HIS ND1	A	/A0320-TYR OH	2.5	SS	9210.8		1296

2pg8.nb	C	/C0069-TYR OH	C	/C0137-HIS ND1	2.5	SS	68	9.8	4039
2pss.nb	C	/C0299-TYR OH	C	/C0304-HIS ND1	2.5	SS	5	6.8	3915
2pv7.nb	B	/B0200-HIS NE2	B	/B0401-TYR OH	2.5	SS	-111.4		2344
2q1w.nb	B	/B0041-HIS NE2	B	/B0294-TYR OH	2.5	SS	-110.4		1958
2q2r.nb	B	/B0221-TYR OH	B	/B0247-HIS ND1	2.5	SS	26	9.6	3694
2q6b.nb	B	/B0635-HIS NE2	B	/B0687-TYR OH	2.5	SS	52	9.9	2558
2q6d.nb	A	/A0159-TYR OH	A	/A0161-HIS ND1	2.5	SS	2	6.9	931
2qby.nb	B	/B0295-HIS ND1	B	/B0316-TYR OH	2.5	SS	21	8.8	2602
2qe3.nb	A	/A0031-HIS ND1	A	/A0083-TYR OH	2.5	SS	-1	9.1	41
2qfv.nb	D	/D0196-HIS ND1	D	/D0237-TYR OH	2.5	SS	41	9.0	5948
2qfw.nb	D	/D0196-HIS ND1	D	/D0237-TYR OH	2.5	SS	41	8.8	5957
2qfx.nb	D	/D0196-HIS ND1	D	/D0237-TYR OH	2.5	SS	41	9.0	5972
2qjr.nb	B	/B0735-TYR OH	B	/B0750-HIS ND1	2.5	SS	15	9.5	5824
2qnv.nb	A	/A0242-HIS NE2	A	/A0306-TYR OH	2.5	SS	6411.5		265
2qps.nb	A	/A0310-TYR OH	A	/A0326-HIS ND1	2.5	SS	16	9.6	1780
2qtk.nb	B	/B0260-HIS ND1	B	/B0307-TYR OH	2.5	SS	47	7.5	2351
2qtr.nb	B	/B0044-HIS ND1	B	/B0112-TYR OH	2.5	SS	68	9.6	1426
2qyh.nb	A	/A0099-HIS ND1	A	/A0158-TYR OH	2.5	SS	5910.8		553
2qyh.nb	C	/C0099-HIS ND1	C	/C0158-TYR OH	2.5	SS	5910.8		3258
2qyw.nb	A	/A0015-HIS NE2	A	/A0084-TYR OH	2.5	SS	6910.8		92
2r0o.nb	A	/A0180-TYR OH	A	/A0203-HIS ND1	2.5	SS	23	9.7	1004
2r0o.nb	B	/B0180-TYR OH	B	/B0203-HIS ND1	2.5	SS	23	9.7	2494
2r5u.nb	C	/C0062-HIS NE2	C	/C0102-TYR OH	2.5	SS	4010.4		1894
2r6d.nb	F	/F0048-HIS NE2	F	/F0088-TYR OH	2.5	SS	4010.4		7874
2r92.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.8		1713
2r9z.nb	A	/A0133-HIS ND1	A	/A0298-TYR OH	2.5	SS	165	7.7	778
2r9z.nb	B	/B0133-HIS ND1	B	/B0298-TYR OH	2.5	SS	165	7.7	3331
2rdb.nb	A	/A0279-TYR OH	A	/A0329-HIS ND1	2.5	SS	50	9.1	1537
2rfc.nb	D	/D0023-HIS ND1	D	/D0269-TYR OH	2.5	SS	-1	7.2	4169
2rfo.nb	B	/B0439-HIS ND1	B	/B0457-TYR OH	2.5	SS	18	8.8	3684
2rfo.nb	B	/B0505-HIS NE2	B	/B0556-TYR OH	2.5	SS	-110.0		3965
2rgk.nb	A	/A0168-TYR OH	A	/A0219-HIS ND1	2.5	SS	51	7.5	804
2rgk.nb	D	/D0168-TYR OH	D	/D0219-HIS ND1	2.5	SS	51	7.5	6313
2rgn.nb	E	/E0217-HIS NE2	E	/E0249-TYR OH	2.5	SS	3212.0		4972
2rip.nb	A	/A0735-TYR OH	A	/A0750-HIS ND1	2.5	SS	15	9.5	2867
2rve.nb	A	/A0072-TYR OH	A	/A0131-HIS ND1	2.5	SS	5910.4		302
2tmd.nb	A	/A0006-HIS ND1	A	/A0339-TYR OH	2.5	SS	33311.4		32
2tsc.nb	B	/B0147-HIS ND1	B	/B0181-TYR OH	2.5	SS	34	9.7	2160
2udp.nb	A	/A0177-TYR OH	A	/A0243-HIS NE2	2.5	SS	6611.1		1326
2up1.nb	A	/A0124-TYR OH	A	/A0168-HIS ND1	2.5	SS	44	7.8	668
2uuw.nb	A	/A0313-HIS NE2	A	/A0351-TYR OH	2.5	SS	3811.3		1657
2ux0.nb	B	/B0418-TYR OH	B	/B0444-HIS ND1	2.5	SS	26	9.8	708
2uy1.nb	A	/A0199-HIS ND1	A	/A0219-TYR OH	2.5	SS	20	8.2	1054
2uye.nb	A	/A0171-TYR OH	A	/A0206-HIS ND1	2.5	SS	35	9.0	520
2v1x.nb	A	/A0554-TYR OH	A	/A0584-HIS NE2	2.5	SS	3011.9		2563
2v3e.nb	A	/A0490-HIS ND1	A	/A0492-TYR OH	2.5	SS	2	6.4	3574
2v7w.nb	B	/B0211-HIS ND1	B	/B0284-TYR OH	2.5	SS	73	9.6	2929
2v9p.nb	A	/A0482-HIS ND1	A	/A0532-TYR OH	2.5	SS	50	9.6	827
2v9p.nb	G	/G0482-HIS ND1	G	/G0532-TYR OH	2.5	SS	50	9.5	7366
2vc2.nb	B	/B0115-TYR OH	B	/B0192-HIS ND1	2.5	SS	7710.1		2300
2vcc.nb	A	/A0092-TYR OH	A	/A0122-HIS NE2	2.5	SS	3011.6		464
2vf0.nb	A	/A0147-HIS ND1	A	/A0181-TYR OH	2.5	SS	34	9.7	702
2viq.nb	A	/A0094-TYR OH	A	/A0099-HIS ND1	2.5	SS	7	7.2	663
2vkp.nb	B	/B0026-HIS ND1	B	/B0070-TYR OH	2.5	SS	44	9.4	767
2vl8.nb	B	/B0185-HIS ND1	B	/B0209-TYR OH	2.5	SS	2410.1		3256
2vn4.nb	A	/A0418-HIS ND1	A	/A0423-TYR OH	2.5	SS	5	7.8	2911

2vpw.nb	A	/A0333-HIS	NE2	A	/A0623-TYR	OH	2.5	SS	29010.6	1576
2vpx.nb	A	/A0333-HIS	NE2	A	/A0623-TYR	OH	2.5	SS	29010.6	1601
2vq0.nb	A	/A0140-HIS	ND1	A	/A0164-TYR	OH	2.5	SS	24 7.2	365
2vt5.nb	D	/D0279-TYR	OH	D	/D0311-HIS	ND1	2.5	SS	32 8.5	5039
2vt5.nb	F	/F0279-TYR	OH	F	/F0311-HIS	ND1	2.5	SS	32 8.7	7646
2vt8.nb	A	/A0027-HIS	ND1	A	/A0069-TYR	OH	2.5	SS	-1 9.3	157
2vt8.nb	B	/B0027-HIS	ND1	B	/B0069-TYR	OH	2.5	SS	-1 9.5	765
2vur.nb	A	/A0307-HIS	ND1	A	/A0349-TYR	OH	2.5	SS	4210.0	1415
2vv1.nb	A	/A0323-HIS	NE2	A	/A0473-TYR	OH	2.5	SS	150 9.7	561
2vvj.nb	C	/C0071-TYR	OH	C	/C0190-HIS	NE2	2.5	SS	11910.2	3560
2vvl.nb	E	/E0086-TYR	OH	E	/E0378-HIS	ND1	2.5	SS	292 9.6	8585
2vwd.nb	A	/A0231-TYR	OH	A	/A0233-HIS	ND1	2.5	SS	2 7.1	303
2vyc.nb	C	/C0315-TYR	OH	C	/C0345-HIS	ND1	2.5	SS	30 7.4	7987
2vyc.nb	F	/F0061-TYR	OH	F	/F0069-HIS	ND1	2.5	SS	8 8.3	16594
2vye.nb	A	/A0048-HIS	NE2	A	/A0088-TYR	OH	2.5	SS	4010.4	193
2w22.nb	A	/A0030-TYR	OH	A	/A0113-HIS	ND1	2.5	SS	83 9.8	251
2w3y.nb	B	/B0175-HIS	ND1	B	/B0187-TYR	OH	2.5	SS	12 6.8	2786
2w9x.nb	A	/A0156-TYR	OH	A	/A0334-HIS	ND1	2.5	SS	178 9.1	622
2wbb.nb	G	/G0279-TYR	OH	G	/G0311-HIS	ND1	2.5	SS	32 8.4	9036
2wbd.nb	B	/B0164-TYR	OH	B	/B0253-HIS	ND1	2.5	SS	89 9.1	1918
2wbd.nb	D	/D0164-TYR	OH	D	/D0253-HIS	ND1	2.5	SS	89 9.0	4487
2wbk.nb	A	/A0488-TYR	OH	A	/A0511-HIS	ND1	2.5	SS	23 9.5	2059
2wc5.nb	A	/A0011-HIS	ND1	A	/A0076-TYR	OH	2.5	SS	6510.4	101
2wc6.nb	A	/A0011-HIS	ND1	A	/A0076-TYR	OH	2.5	SS	6510.4	101
2wc7.nb	A	/A0087-TYR	OH	A	/A0322-HIS	NE2	2.5	SS	23511.8	497
2wcs.nb	A	/A0087-TYR	OH	A	/A0322-HIS	NE2	2.5	SS	23512.1	449
2wde.nb	A	/A0370-HIS	NE2	A	/A0433-TYR	OH	2.5	SS	6311.4	2315
2wiu.nb	C	/C0389-HIS	ND1	C	/C0437-TYR	OH	2.5	SS	48 8.6	4238
2wjs.nb	A	/A2581-TYR	OH	A	/A2594-HIS	ND1	2.5	SS	13 7.4	1852
2wk8.nb	A	/A0049-TYR	OH	A	/A0205-HIS	ND1	2.5	SS	156 8.6	235
2wka.nb	A	/A0049-TYR	OH	A	/A0205-HIS	ND1	2.5	SS	156 8.6	294
2wkg.nb	A	/A0087-TYR	OH	A	/A0322-HIS	NE2	2.5	SS	23512.0	421
2wpw.nb	B	/B0180-TYR	OH	B	/B0275-HIS	ND1	2.5	SS	-110.0	1941
2wpw.nb	D	/D0180-TYR	OH	D	/D0275-HIS	ND1	2.5	SS	-110.1	4339
2wr1.nb	B	/B0351-TYR	OH	B	/B0440-HIS	ND1	2.5	SS	89 8.8	3379
2wr7.nb	B	/B0351-TYR	OH	B	/B0440-HIS	ND1	2.5	SS	89 8.7	3219
2wrd.nb	A	/A0471-HIS	NE2	A	/A0486-TYR	OH	2.5	SS	1512.7	1753
2wrd.nb	B	/B0471-HIS	NE2	B	/B0486-TYR	OH	2.5	SS	1512.8	3653
2wrf.nb	G	/G0471-HIS	NE2	G	/G0486-TYR	OH	2.5	SS	1513.0	12872
2wv0.nb	I	/I0107-TYR	OH	I	/I0129-HIS	ND1	2.5	SS	22 7.4	7408
2wvz.nb	D	/D0669-TYR	OH	D	/D0720-HIS	ND1	2.5	SS	51 7.4	12791
2ww3.nb	E	/E0669-TYR	OH	E	/E0720-HIS	ND1	2.5	SS	51 7.4	16223
2wyi.nb	B	/B0689-HIS	NE2	B	/B0741-TYR	OH	2.5	SS	5211.5	6949
2x6t.nb	A	/A0102-HIS	NE2	A	/A0150-TYR	OH	2.5	SS	4811.2	477
2x6t.nb	C	/C0102-HIS	NE2	C	/C0150-TYR	OH	2.5	SS	4811.2	3089
2x6t.nb	E	/E0102-HIS	NE2	E	/E0150-TYR	OH	2.5	SS	4811.2	5699
2x6t.nb	G	/G0102-HIS	NE2	G	/G0150-TYR	OH	2.5	SS	4811.2	8311
2x6t.nb	H	/H0102-HIS	NE2	H	/H0150-TYR	OH	2.5	SS	4811.1	9623
2x6t.nb	J	/J0102-HIS	NE2	J	/J0150-TYR	OH	2.5	SS	4811.2	12231
2ysu.nb	A	/A0477-HIS	ND1	A	/A0505-TYR	OH	2.5	SS	28 7.3	1804
2yu9.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.5	SS	2012.7	1562
2yw7.nb	B	/B0028-TYR	OH	B	/B0141-HIS	ND1	2.5	SS	11310.2	731
2yw7.nb	F	/F0028-TYR	OH	F	/F0141-HIS	ND1	2.5	SS	11310.2	3173
2yxu.nb	A	/A0079-TYR	OH	A	/A0246-HIS	ND1	2.5	SS	-1 9.7	441
2z0q.nb	A	/A0067-HIS	NE2	A	/A0101-TYR	OH	2.5	SS	3411.6	431
2z5g.nb	A	/A0029-TYR	OH	A	/A0112-HIS	ND1	2.5	SS	8310.2	242

2z8w.nb	A	/A0202-TYR OH	A	/A0220-HIS ND1	2.5	SS	18	9.0		605
2z9f.nb	A	/A0087-HIS ND1	A	/A0112-TYR OH	2.5	SS	2510.0			456
2z9f.nb	C	/C0087-HIS ND1	C	/C0112-TYR OH	2.5	SS	2510.0			1949
2zbk.nb	F	/F0099-TYR OH	F	/F0348-HIS NE2	2.5	SS	24911.3			7623
2zc7.nb	B	/B0314-HIS ND1	B	/B0325-TYR OH	2.5	SS	11	7.6		2932
2ze3.nb	A	/A0089-HIS ND1	A	/A0123-TYR OH	2.5	SS	34	8.9		574
2zjc.nb	A	/A0015-HIS ND1	A	/A0059-TYR OH	2.5	SS	44	9.2		42
2zjc.nb	C	/C0015-HIS ND1	C	/C0059-TYR OH	2.5	SS	44	9.2		1118
2zk3.nb	A	/A0323-HIS NE2	A	/A0473-TYR OH	2.5	SS	150	9.9		596
2zku.nb	C	/C0103-TYR OH	C	/C0118-HIS ND1	2.5	SS	15	9.2		5329
2zku.nb	D	/D0103-TYR OH	D	/D0118-HIS ND1	2.5	SS	15	9.3		7749
2zmj.nb	A	/A0225-HIS NE2	A	/A0291-TYR OH	2.5	SS	6610.9			232
2znh.nb	A	/A0120-HIS ND1	A	/A0166-TYR OH	2.5	SS	-1	8.3		508
2zw9.nb	B	/B0249-HIS NE2	B	/B0351-TYR OH	2.5	SS	102	8.4		3727
2zwy.nb	B	/B0243-TYR OH	B	/B0259-HIS NE2	2.5	SS	1612.5			3411
2zzc.nb	D	/D0380-TYR OH	D	/D0439-HIS ND1	2.5	SS	59	7.3		7203
3a29.nb	B	/B0279-TYR OH	B	/B0311-HIS ND1	2.5	SS	32	8.5		2753
3a29.nb	C	/C0279-TYR OH	C	/C0311-HIS ND1	2.5	SS	32	8.4		4239
3a29.nb	D	/D0164-TYR OH	D	/D0253-HIS ND1	2.5	SS	89	9.0		5112
3abk.nb	A	/A0261-TYR OH	A	/A0395-HIS ND1	2.5	SS	134	9.8		1331
3abl.nb	A	/A0261-TYR OH	A	/A0395-HIS ND1	2.5	SS	134	9.9		1334
3b5q.nb	A	/A0398-HIS ND1	A	/A0448-TYR OH	2.5	SS	5010.4			2367
3b7p.nb	A	/A0299-TYR OH	A	/A0304-HIS ND1	2.5	SS	5	6.7		1546
3bba.nb	B	/B0199-TYR OH	B	/B0226-HIS ND1	2.5	SS	2710.2			1377
3bcc.nb	C	/C0108-TYR OH	C	/C0309-HIS ND1	2.5	SS	201	9.0		3856
3bji.nb	A	/A0247-HIS NE2	A	/A0280-TYR OH	2.5	SS	3311.7			318
3bnb.nb	A	/A0290-HIS ND1	A	/A0293-TYR OH	2.5	SS	3	6.0		1845
3bnd.nb	A	/A0290-HIS ND1	A	/A0293-TYR OH	2.5	SS	3	6.1		1757
3bne.nb	A	/A0290-HIS ND1	A	/A0293-TYR OH	2.5	SS	3	6.0		1810
3bng.nb	A	/A0040-HIS NE2	A	/A0057-TYR OH	2.5	SS	1710.9			27
3bny.nb	A	/A0043-HIS ND1	A	/A0126-TYR OH	2.5	SS	83	9.4		190
3br9.nb	A	/A0103-TYR OH	A	/A0118-HIS ND1	2.5	SS	15	9.3		671
3brh.nb	A	/A0142-TYR OH	A	/A0226-HIS NE2	2.5	SS	-112.3			909
3bs5.nb	B	/B0135-TYR OH	B	/B0167-HIS ND1	2.5	SS	32	9.7		642
3bsc.nb	A	/A0176-TYR OH	A	/A0562-HIS NE2	2.5	SS	38612.2			940
3bsh.nb	A	/A0316-HIS NE2	A	/A0364-TYR OH	2.5	SS	4812.3			1569
3btv.nb	A	/A0118-TYR OH	A	/A0376-HIS ND1	2.5	SS	-110.0			519
3c1i.nb	A	/A0064-TYR OH	A	/A0100-HIS ND1	2.5	SS	36	9.3		428
3c6v.nb	B	/B0029-TYR OH	B	/B0068-HIS NE2	2.5	SS	3911.5			1306
3c7p.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.7			828
3c7v.nb	D	/D0041-HIS NE2	D	/D0050-TYR OH	2.5	SS	913.0			3585
3c8k.nb	D	/D0142-TYR OH	D	/D0189-HIS NE2	2.5	SS	4712.7			1476
3ca2.nb	A	/A0107-HIS NE2	A	/A0194-TYR OH	2.5	SS	8611.7			718
3ccb.nb	D	/D0735-TYR OH	D	/D0750-HIS ND1	2.5	SS	15	9.4		11945
3cde.nb	A	/A0176-TYR OH	A	/A0562-HIS NE2	2.5	SS	38612.3			1078
3cgn.nb	A	/A0029-TYR OH	A	/A0031-HIS ND1	2.5	SS	2	6.1		142
3cic.nb	A	/A0242-HIS ND1	A	/A0245-TYR OH	2.5	SS	3	6.0		1424
3ciz.nb	A	/A0176-TYR OH	A	/A0562-HIS NE2	2.5	SS	38612.2			1218
3ciz.nb	B	/B0176-TYR OH	B	/B0562-HIS NE2	2.5	SS	38612.2			4959
3cj0.nb	A	/A0176-TYR OH	A	/A0562-HIS NE2	2.5	SS	38612.5			1064
3cj0.nb	B	/B0176-TYR OH	B	/B0562-HIS NE2	2.5	SS	38612.4			4327
3cj4.nb	B	/B0103-TYR OH	B	/B0118-HIS ND1	2.5	SS	15	9.3		3881
3cj4.nb	B	/B0176-TYR OH	B	/B0562-HIS NE2	2.5	SS	38612.2			4276
3cj5.nb	A	/A0176-TYR OH	A	/A0562-HIS NE2	2.5	SS	38612.0			1123
3cjx.nb	H	/H0069-HIS ND1	H	/H0092-TYR OH	2.5	SS	23	7.4		4633
3cl8.nb	B	/B0133-TYR OH	B	/B0144-HIS ND1	2.5	SS	1110.1			2138

3cmm.nb	C	/C0293-HIS	ND1	C	/C0390-TYR	OH	2.5	SS	97	7.5	5364
3cr9.nb	A	/A0192-TYR	OH	A	/A0253-HIS	NE2	2.5	SS	6112.6		920
3cru.nb	A	/A0031-HIS	ND1	A	/A0057-TYR	OH	2.5	SS	26	9.2	199
3csu.nb	B	/B0156-HIS	ND1	B	/B0185-TYR	OH	2.5	SS	29	7.6	2749
3csv.nb	A	/A0124-HIS	ND1	A	/A0246-TYR	OH	2.5	SS	12210.7		678
3cty.nb	A	/A0128-HIS	ND1	A	/A0144-TYR	OH	2.5	SS	16	8.7	570
3cvv.nb	A	/A0369-HIS	ND1	A	/A0423-TYR	OH	2.5	SS	54	7.9	2700
3cwb.nb	P	/P0108-TYR	OH	P	/P0309-HIS	ND1	2.5	SS	201	9.1	11585
3cwe.nb	A	/A0624-TYR	OH	A	/A0714-HIS	NE2	2.5	SS	9012.1		1050
3d1j.nb	A	/A0134-HIS	ND1	A	/A0473-TYR	OH	2.5	SS	339	9.4	594
3d2u.nb	A	/A0007-TYR	OH	A	/A0100-HIS	NE2	2.5	SS	93	9.0	68
3d3a.nb	A	/A0051-TYR	OH	A	/A0083-HIS	NE2	2.5	SS	3211.8		201
3d3l.nb	A	/A0191-TYR	OH	A	/A0425-HIS	ND1	2.5	SS	-111.5		86
3d4x.nb	C	/C0024-TYR	OH	C	/C0113-HIS	NE2	2.5	SS	8910.9		1548
3d5m.nb	B	/B0103-TYR	OH	B	/B0118-HIS	ND1	2.5	SS	15	9.1	3670
3d66.nb	A	/A0175-HIS	NE2	A	/A0186-TYR	OH	2.5	SS	11	9.4	832
3d66.nb	B	/B0175-HIS	NE2	B	/B0186-TYR	OH	2.5	SS	11	9.4	2557
3d66.nb	C	/C0175-HIS	NE2	C	/C0186-TYR	OH	2.5	SS	11	9.3	4262
3dby.nb	J	/J0133-HIS	ND1	J	/J0242-TYR	OH	2.5	SS	109	8.4	11436
3dby.nb	O	/O0133-HIS	ND1	O	/O0242-TYR	OH	2.5	SS	109	8.2	17379
3dca.nb	A	/A0038-TYR	OH	A	/A0115-HIS	ND1	2.5	SS	-1	7.7	177
3dca.nb	B	/B0038-TYR	OH	B	/B0115-HIS	ND1	2.5	SS	-1	7.8	635
3dca.nb	C	/C0038-TYR	OH	C	/C0115-HIS	ND1	2.5	SS	-1	7.7	1096
3dca.nb	D	/D0038-TYR	OH	D	/D0115-HIS	ND1	2.5	SS	-1	7.7	1547
3dev.nb	A	/A0021-HIS	NE2	A	/A0074-TYR	OH	2.5	SS	5312.3		111
3dev.nb	B	/B0021-HIS	NE2	B	/B0074-TYR	OH	2.5	SS	5312.3		1421
3dl5.nb	E	/E0403-HIS	ND1	E	/E0438-TYR	OH	2.5	SS	35	9.4	9800
3dmq.nb	A	/A0349-TYR	OH	A	/A0411-HIS	ND1	2.5	SS	62	9.0	1394
3dmq.nb	B	/B0349-TYR	OH	B	/B0411-HIS	ND1	2.5	SS	-1	9.0	4982
3dty.nb	B	/B0029-HIS	ND1	B	/B0337-TYR	OH	2.5	SS	-1	8.5	1685
3dty.nb	D	/D0177-HIS	ND1	D	/D0201-TYR	OH	2.5	SS	-111.5		3914
3dty.nb	E	/E0177-HIS	ND1	E	/E0201-TYR	OH	2.5	SS	-111.4		5421
3du5.nb	A	/A0339-HIS	ND1	A	/A0389-TYR	OH	2.5	SS	50	9.3	1518
3du5.nb	B	/B0339-HIS	ND1	B	/B0389-TYR	OH	2.5	SS	50	9.8	4068
3dws.nb	B	/B0146-HIS	ND1	B	/B0161-TYR	OH	2.5	SS	15	9.2	2931
3dx9.nb	A	/A0052-TYR	OH	A	/A0055-HIS	ND1	2.5	SS	3	8.7	230
3dx9.nb	C	/C0052-TYR	OH	C	/C0055-HIS	ND1	2.5	SS	3	8.7	2007
3dxp.nb	A	/A0257-HIS	NE2	A	/A0287-TYR	OH	2.5	SS	3011.0		1159
3dy5.nb	C	/C0789-HIS	NE2	C	/C1013-TYR	OH	2.5	SS	-1	9.9	7131
3dyo.nb	D	/D0357-HIS	ND1	D	/D0392-TYR	OH	2.5	SS	35	8.7	14178
3e04.nb	B	/B0204-HIS	NE2	B	/B0270-TYR	OH	2.5	SS	6612.0		2763
3e0o.nb	D	/D0036-HIS	ND1	D	/D0042-TYR	OH	2.5	SS	610.8		2126
3e1k.nb	G	/G0036-HIS	ND1	G	/G0385-TYR	OH	2.5	SS	-1	8.8	5027
3e1k.nb	K	/K0118-TYR	OH	K	/K0392-HIS	ND1	2.5	SS	-1	9.8	8608
3e1k.nb	M	/M0036-HIS	ND1	M	/M0385-TYR	OH	2.5	SS	-1	8.8	9899
3e3k.nb	A	/A0022-TYR	OH	A	/A0098-HIS	ND1	2.5	SS	76	9.7	118
3e7n.nb	A	/A0081-HIS	NE2	A	/A0103-TYR	OH	2.5	SS	2211.6		390
3e7n.nb	D	/D0081-HIS	NE2	D	/D0103-TYR	OH	2.5	SS	2211.7		2014
3e7n.nb	E	/E0081-HIS	NE2	E	/E0103-TYR	OH	2.5	SS	2211.7		2552
3e7n.nb	K	/K0081-HIS	NE2	K	/K0103-TYR	OH	2.5	SS	2211.6		5745
3e7n.nb	N	/N0081-HIS	NE2	N	/N0103-TYR	OH	2.5	SS	2211.7		7283
3ebl.nb	B	/B0126-HIS	NE2	B	/B0254-TYR	OH	2.5	SS	-1	9.9	1813
3ebl.nb	C	/C0126-HIS	NE2	C	/C0254-TYR	OH	2.5	SS	-1	9.9	3110
3ebl.nb	D	/D0126-HIS	NE2	D	/D0254-TYR	OH	2.5	SS	128	9.9	4418
3ebl.nb	D	/D0205-HIS	ND1	D	/D0305-TYR	OH	2.5	SS	10010.4		4752
3ebl.nb	E	/E0126-HIS	NE2	E	/E0254-TYR	OH	2.5	SS	-1	9.9	5763

3ed1.nb	B	/B0126-HIS	NE2	B	/B0254-TYR	OH	2.5	SS	-1 9.8	1818
3egq.nb	B	/B0022-HIS	NE2	B	/B0094-TYR	OH	2.5	SS	7210.3	828
3eh7.nb	A	/A0262-HIS	NE2	A	/A0294-TYR	OH	2.5	SS	3212.4	1485
3eic.nb	A	/A0053-HIS	ND1	A	/A0058-TYR	OH	2.5	SS	5 8.3	349
3eic.nb	F	/F0053-HIS	ND1	F	/F0058-TYR	OH	2.5	SS	5 8.0	3713
3eip.nb	A	/A0064-HIS	NE2	A	/A0073-TYR	OH	2.5	SS	911.5	360
3ela.nb	H	/H0241-HIS	ND1	H	/H0383-TYR	OH	2.5	SS	142 9.1	1010
3enc.nb	B	/B0031-HIS	ND1	B	/B0069-TYR	OH	2.5	SS	38 7.7	416
3enk.nb	B	/B0180-TYR	OH	B	/B0246-HIS	NE2	2.5	SS	6610.8	3204
3eoq.nb	A	/A0138-TYR	OH	A	/A0297-HIS	ND1	2.5	SS	159 9.3	816
3err.nb	A	/A0251-TYR	OH	A	/A0276-HIS	ND1	2.5	SS	25 7.5	1710
3err.nb	B	/B0251-TYR	OH	B	/B0276-HIS	ND1	2.5	SS	25 7.6	4159
3es9.nb	A	/A0302-HIS	ND1	A	/A0575-TYR	OH	2.5	SS	-1 9.5	965
3es9.nb	B	/B0392-TYR	OH	B	/B0443-HIS	ND1	2.5	SS	5110.7	3367
3eu4.nb	A	/A0067-TYR	OH	A	/A0129-HIS	ND1	2.5	SS	62 8.5	200
3eyk.nb	A	/A0176-TYR	OH	A	/A0259-HIS	NE2	2.5	SS	8311.2	1006
3eym.nb	A	/A0183-HIS	ND1	A	/A0195-TYR	OH	2.5	SS	1210.2	789
3ez3.nb	B	/B0196-HIS	NE2	B	/B0206-TYR	OH	2.5	SS	1012.0	2367
3ezu.nb	A	/A0030-HIS	ND1	A	/A0094-TYR	OH	2.5	SS	6411.3	221
3f1f.nb	S	/S0034-HIS	ND1	S	/S0036-TYR	OH	2.5	SS	2 6.9	6739
3f1h.nb	S	/S0034-HIS	ND1	S	/S0036-TYR	OH	2.5	SS	2 7.0	6752
3f69.nb	A	/A0200-TYR	OH	A	/A0228-HIS	ND1	2.5	SS	2810.1	766
3f8e.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7111.8	358
3f8n.nb	B	/B0092-TYR	OH	B	/B0128-HIS	NE2	2.5	SS	3610.6	829
3f9r.nb	B	/B0082-HIS	NE2	B	/B0190-TYR	OH	2.5	SS	10811.2	2198
3f9s.nb	A	/A0035-TYR	OH	A	/A0125-HIS	ND1	2.5	SS	90 8.0	287
3fal.nb	B	/B0254-HIS	NE2	B	/B0319-TYR	OH	2.5	SS	6511.8	1068
3fbb.nb	A	/A0053-HIS	ND1	A	/A0058-TYR	OH	2.5	SS	5 8.2	343
3fbb.nb	B	/B0053-HIS	ND1	B	/B0058-TYR	OH	2.5	SS	5 8.2	987
3fbb.nb	F	/F0053-HIS	ND1	F	/F0058-TYR	OH	2.5	SS	5 7.9	3617
3fbc.nb	E	/E0053-HIS	ND1	E	/E0058-TYR	OH	2.5	SS	5 8.3	2747
3fbc.nb	F	/F0053-HIS	ND1	F	/F0058-TYR	OH	2.5	SS	5 7.9	3361
3fbe.nb	F	/F0053-HIS	ND1	F	/F0058-TYR	OH	2.5	SS	5 8.1	3519
3fbr.nb	A	/A0389-HIS	ND1	A	/A0437-TYR	OH	2.5	SS	48 8.3	1595
3fc6.nb	B	/B0254-HIS	NE2	B	/B0319-TYR	OH	2.5	SS	6511.9	1239
3fcw.nb	A	/A0053-HIS	ND1	A	/A0058-TYR	OH	2.5	SS	5 8.4	341
3fg4.nb	C	/C0581-HIS	ND1	C	/C0584-TYR	OH	2.5	SS	3 6.2	6741
3fg4.nb	C	/C0789-HIS	NE2	C	/C1013-TYR	OH	2.5	SS	-1 9.8	7735
3fg4.nb	D	/D0581-HIS	ND1	D	/D0584-TYR	OH	2.5	SS	3 6.2	9694
3fhs.nb	A	/A0059-HIS	ND1	A	/A0073-TYR	OH	2.5	SS	14 9.9	320
3fhx.nb	B	/B0079-TYR	OH	B	/B0246-HIS	ND1	2.5	SS	16710.0	1908
3fi8.nb	A	/A0138-HIS	ND1	A	/A0187-TYR	OH	2.5	SS	-1 8.9	294
3fi8.nb	A	/A0213-HIS	ND1	A	/A0357-TYR	OH	2.5	SS	144 9.5	685
3fjk.nb	A	/A0001EHIS	ND1	A	/A0125-TYR	OH	2.5	SS	12610.7	16
3fjv.nb	A	/A0022-HIS	ND1	A	/A0052-TYR	OH	2.5	SS	30 8.2	182
3fku.nb	J	/J0022-TYR	OH	J	/J0111-HIS	ND1	2.5	SS	89 9.0	8434
3flb.nb	A	/A0129-TYR	OH	A	/A0182-HIS	ND1	2.5	SS	5310.0	831
3fn9.nb	B	/B0062-HIS	ND1	B	/B0083-TYR	OH	2.5	SS	2110.2	2918
3fn9.nb	C	/C0062-HIS	ND1	C	/C0083-TYR	OH	2.5	SS	2110.3	5629
3fn9.nb	C	/C0537-HIS	ND1	C	/C0594-TYR	OH	2.5	SS	57 8.4	7666
3fo5.nb	A	/A0455-HIS	NE2	A	/A0557-TYR	OH	2.5	SS	10211.3	662
3fpx.nb	A	/A0216-HIS	NE2	A	/A0281-TYR	OH	2.5	SS	6512.3	1469
3frz.nb	A	/A0176-TYR	OH	A	/A0562-HIS	NE2	2.5	SS	38612.0	1342
3fvr.nb	C	/C0049-TYR	OH	C	/C0100-HIS	ND1	2.5	SS	51 9.2	2963
3fvr.nb	H	/H0049-TYR	OH	H	/H0100-HIS	ND1	2.5	SS	51 9.2	9804
3fvr.nb	M	/M0049-TYR	OH	M	/M0100-HIS	ND1	2.5	SS	51 9.2	13879

3fvt.nb	H	/H0049-TYR OH	H	/H0100-HIS ND1	2.5	SS	51	9.1	9801
3fvv.nb	A	/A0104-HIS NE2	A	/A0184-TYR OH	2.5	SS	8011.8		593
3fy4.nb	B	/B0368-HIS ND1	B	/B0422-TYR OH	2.5	SS	54	8.1	3902
3fyt.nb	A	/A0049-TYR OH	A	/A0100-HIS ND1	2.5	SS	51	9.3	211
3fyt.nb	C	/C0049-TYR OH	C	/C0100-HIS ND1	2.5	SS	51	9.3	2909
3fyt.nb	D	/D0049-TYR OH	D	/D0100-HIS ND1	2.5	SS	51	9.3	4263
3fyt.nb	F	/F0049-TYR OH	F	/F0100-HIS ND1	2.5	SS	51	9.3	6941
3fyt.nb	H	/H0049-TYR OH	H	/H0100-HIS ND1	2.5	SS	51	9.1	9629
3fyu.nb	C	/C0049-TYR OH	C	/C0100-HIS ND1	2.5	SS	51	9.0	3029
3fyu.nb	F	/F0049-TYR OH	F	/F0100-HIS ND1	2.5	SS	51	9.1	7208
3fzb.nb	F	/F0006-HIS NE2	F	/F0132-TYR OH	2.5	SS	-1	9.6	2514
3g2x.nb	A	/A0053-HIS ND1	A	/A0058-TYR OH	2.5	SS	5	8.5	300
3g3s.nb	A	/A0166-HIS ND1	A	/A0194-TYR OH	2.5	SS	28	9.5	1242
3g8r.nb	A	/A0047-TYR OH	A	/A0110-HIS ND1	2.5	SS	6311.4		229
3g8r.nb	B	/B0047-TYR OH	B	/B0110-HIS ND1	2.5	SS	6311.2		1574
3ga1.nb	B	/B0044-HIS ND1	B	/B0086-TYR OH	2.5	SS	42	9.8	781
3gbm.nb	C	/C0183-HIS ND1	C	/C0195-TYR OH	2.5	SS	1210.4		2630
3gfg.nb	A	/A0029-HIS ND1	A	/A0314-TYR OH	2.5	SS	-1	9.2	121
3gfg.nb	C	/C0029-HIS ND1	C	/C0314-TYR OH	2.5	SS	-1	9.2	2903
3gfg.nb	D	/D0029-HIS ND1	D	/D0314-TYR OH	2.5	SS	-1	9.1	4278
3gfg.nb	J	/J0029-HIS ND1	J	/J0314-TYR OH	2.5	SS	-1	9.4	12500
3gfg.nb	L	/L0029-HIS ND1	L	/L0314-TYR OH	2.5	SS	-1	9.3	15215
3glg.nb	G	/G0328-TYR OH	G	/G0360-HIS NE2	2.5	SS	32	8.4	9863
3gn6.nb	B	/B0052-HIS NE2	B	/B0115-TYR OH	2.5	SS	6310.4		2159
3gn6.nb	D	/D0052-HIS NE2	D	/D0115-TYR OH	2.5	SS	6310.3		5095
3go4.nb	A	/A0095-HIS ND1	A	/A0109-TYR OH	2.5	SS	-1	9.0	618
3gpa.nb	A	/A0053-HIS ND1	A	/A0058-TYR OH	2.5	SS	5	8.2	365
3gpa.nb	F	/F0053-HIS ND1	F	/F0058-TYR OH	2.5	SS	5	8.0	3996
3gqo.nb	D	/D0064-HIS ND1	D	/D0101-TYR OH	2.5	SS	37	9.9	2698
3gtp.nb	A	/A0458-HIS NE2	A	/A0478-TYR OH	2.5	SS	2012.7		1580
3h14.nb	A	/A0085-TYR OH	A	/A0204-HIS ND1	2.5	SS	11910.7		454
3h1h.nb	O	/O0164-HIS NE2	O	/O0316-TYR OH	2.5	SS	15211.7		10261
3h1i.nb	B	/B0164-HIS NE2	B	/B0316-TYR OH	2.5	SS	15211.6		2460
3h1i.nb	C	/C0108-TYR OH	C	/C0309-HIS ND1	2.5	SS	201	9.1	3962
3h1i.nb	O	/O0164-HIS NE2	O	/O0316-TYR OH	2.5	SS	15211.6		10214
3h1i.nb	P	/P0108-TYR OH	P	/P0309-HIS ND1	2.5	SS	201	9.1	11710
3h1k.nb	B	/B0254-HIS ND1	B	/B0325-TYR OH	2.5	SS	71	7.2	2790
3h3v.nb	C	/C0657-HIS ND1	C	/C0679-TYR OH	2.5	SS	-1	8.7	7858
3h3v.nb	L	/L0040-HIS ND1	L	/L0061-TYR OH	2.5	SS	21	8.9	14108
3h3x.nb	A	/A0243-HIS NE2	A	/A0261-TYR OH	2.5	SS	18	9.7	975
3h3x.nb	S	/S0289-TYR OH	S	/S0419-HIS ND1	2.5	SS	13010.4		9391
3h5u.nb	B	/B0103-TYR OH	B	/B0118-HIS ND1	2.5	SS	15	9.1	4035
3h7l.nb	A	/A0285-HIS NE2	A	/A0293-TYR OH	2.5	SS	811.3		1376
3h8m.nb	A	/A0940-TYR OH	A	/A0973-HIS ND1	2.5	SS	33	9.9	132
3h98.nb	A	/A0176-TYR OH	A	/A0562-HIS NE2	2.5	SS	-112.5		1218
3h98.nb	B	/B0103-TYR OH	B	/B0118-HIS ND1	2.5	SS	15	9.2	4403
3h99.nb	A	/A0028-HIS ND1	A	/A0091-TYR OH	2.5	SS	63	9.7	267
3hae.nb	L	/L0191-HIS ND1	L	/L0194-TYR OH	2.5	SS	3	7.5	6237
3ham.nb	B	/B0121-HIS ND1	B	/B0246-TYR OH	2.5	SS	12510.2		2180
3hdq.nb	I	/I0063-HIS NE2	I	/I0082-TYR OH	2.5	SS	1912.5		12134
3he1.nb	C	/C0065-HIS ND1	C	/C0148-TYR OH	2.5	SS	-1	9.2	1830
3he1.nb	E	/E0065-HIS ND1	E	/E0148-TYR OH	2.5	SS	-1	9.2	3386
3hi1.nb	G	/G0249-HIS ND1	G	/G0486-TYR OH	2.5	SS	-1	9.9	314
3hi1.nb	J	/J0249-HIS ND1	J	/J0486-TYR OH	2.5	SS	-110.0		2872
3hkt.nb	A	/A0051-TYR OH	A	/A0122-HIS NE2	2.5	SS	7111.7		345
3hkz.nb	A	/A0433-HIS NE2	A	/A0453-TYR OH	2.5	SS	2012.8		1492

3hox.nb	B	/B0657-HIS	ND1	B	/B0679-TYR	OH	2.5	SS	-1	8.6	7979
3hoy.nb	C	/C0180-TYR	OH	C	/C0188-HIS	ND1	2.5	SS	810.1		10483
3hoy.nb	K	/K0040-HIS	ND1	K	/K0061-TYR	OH	2.5	SS	21	8.9	14285
3hri.nb	A	/A0075-HIS	ND1	A	/A0148-TYR	OH	2.5	SS	-1	8.8	127
3hri.nb	B	/B0075-HIS	ND1	B	/B0148-TYR	OH	2.5	SS	-1	8.7	1660
3hri.nb	E	/E0075-HIS	ND1	E	/E0148-TYR	OH	2.5	SS	-1	8.8	6218
3hri.nb	F	/F0075-HIS	ND1	F	/F0148-TYR	OH	2.5	SS	-1	8.7	7747
3hrs.nb	A	/A0159-HIS	NE2	A	/A0211-TYR	OH	2.5	SS	52	8.4	699
3hrw.nb	C	/C0024-TYR	OH	C	/C0113-HIS	NE2	2.5	SS	8911.1		1351
3hy1.nb	B	/B0020-HIS	NE2	B	/B0101-TYR	OH	2.5	SS	8111.1		2177
3i1n.nb	J	/J0125-TYR	OH	J	/J0132-HIS	NE2	2.5	SS	711.3		4867
3i1p.nb	1	/10018-HIS	ND1	1	/10048-TYR	OH	2.5	SS	3010.3		10268
3i1r.nb	J	/J0125-TYR	OH	J	/J0132-HIS	NE2	2.5	SS	711.2		4822
3i2e.nb	B	/B0224-TYR	OH	B	/B0232-HIS	ND1	2.5	SS	8	7.4	3263
3i4m.nb	K	/K0040-HIS	ND1	K	/K0061-TYR	OH	2.5	SS	21	9.1	14532
3i4x.nb	A	/A0012-TYR	OH	A	/A0031-HIS	ND1	2.5	SS	19	8.5	85
3ib2.nb	A	/A0526-TYR	OH	A	/A0595-HIS	NE2	2.5	SS	6912.6		1122
3iex.nb	C	/C0137-HIS	ND1	C	/C0168-TYR	OH	2.5	SS	31	8.8	4323
3if2.nb	B	/B0188-TYR	OH	B	/B0409-HIS	NE2	2.5	SS	22111.9		3145
3ion.nb	A	/A0197-HIS	ND1	A	/A0333-TYR	OH	2.5	SS	-1	9.7	600
3iwz.nb	A	/A0218-HIS	ND1	A	/A0227-TYR	OH	2.5	SS	9	8.4	993
3jqp.nb	E	/E0037-HIS	ND1	E	/E0225-TYR	OH	2.5	SS	-1	8.9	4235
3jsa.nb	A	/A0142-TYR	OH	A	/A0225-HIS	ND1	2.5	SS	-110.1		878
3jtq.nb	B	/B0224-HIS	NE2	B	/B0264-TYR	OH	2.5	SS	4011.8		2182
3jyg.nb	C	/C0094-HIS	ND1	C	/C0127-TYR	OH	2.5	SS	33	9.2	2578
3k2h.nb	B	/B0036-HIS	ND1	B	/B0179-TYR	OH	2.5	SS	14310.2		3417
3k2h.nb	B	/B0394-HIS	ND1	B	/B0428-TYR	OH	2.5	SS	34	9.6	5596
3k48.nb	B	/B0110-HIS	ND1	B	/B0157-TYR	OH	2.5	SS	47	9.3	504
3k70.nb	B	/B1119-HIS	ND1	B	/B1129-TYR	OH	2.5	SS	10	9.5	4410
3k70.nb	E	/E1119-HIS	ND1	E	/E1129-TYR	OH	2.5	SS	10	9.5	15697
3k7a.nb	A	/A0458-HIS	NE2	A	/A0478-TYR	OH	2.5	SS	2012.8		1678
3kb6.nb	A	/A0204-TYR	OH	A	/A0209-HIS	ND1	2.5	SS	5	6.4	910
3kb6.nb	C	/C0204-TYR	OH	C	/C0209-HIS	ND1	2.5	SS	5	6.6	3688
3kb6.nb	D	/D0204-TYR	OH	D	/D0209-HIS	ND1	2.5	SS	5	6.4	5066
3kbz.nb	B	/B0279-TYR	OH	B	/B0311-HIS	ND1	2.5	SS	32	8.5	2665
3kbz.nb	D	/D0279-TYR	OH	D	/D0311-HIS	ND1	2.5	SS	32	8.4	5509
3kc0.nb	B	/B0164-TYR	OH	B	/B0253-HIS	ND1	2.5	SS	89	9.0	2131
3kct.nb	A	/A0075-HIS	NE2	A	/A0193-TYR	OH	2.5	SS	118	9.9	546
3kfc.nb	A	/A0270-HIS	NE2	A	/A0335-TYR	OH	2.5	SS	6511.8		218
3kls.nb	A	/A0129-HIS	ND1	A	/A0146-TYR	OH	2.5	SS	17	7.3	412
3kls.nb	A	/A1124-TYR	OH	A	/A1421-HIS	ND1	2.5	SS	-1	6.8	4101
3kls.nb	B	/B1124-TYR	OH	B	/B1421-HIS	ND1	2.5	SS	-1	6.8	10758
3km4.nb	A	/A0191-HIS	ND1	A	/A0277-TYR	OH	2.5	SS	8610.8		1125
3km9.nb	B	/B0129-HIS	ND1	B	/B0146-TYR	OH	2.5	SS	17	7.5	6090
3km9.nb	B	/B1124-TYR	OH	B	/B1421-HIS	ND1	2.5	SS	-1	7.0	9679
3kop.nb	B	/B0044-HIS	NE2	B	/B0114-TYR	OH	2.5	SS	-110.9		1281
3kq0.nb	A	/A0065-TYR	OH	A	/A0172-HIS	ND1	2.5	SS	10711.0		476
3kqx.nb	A	/A0356-HIS	ND1	A	/A0472-TYR	OH	2.5	SS	11610.1		1135
3l70.nb	B	/B0164-HIS	NE2	B	/B0316-TYR	OH	2.5	SS	15211.7		2537
3l70.nb	B	/B0254-HIS	ND1	B	/B0325-TYR	OH	2.5	SS	71	7.3	2858
3l70.nb	O	/O0164-HIS	NE2	O	/O0316-TYR	OH	2.5	SS	15211.6		10459
3l70.nb	O	/O0254-HIS	ND1	O	/O0325-TYR	OH	2.5	SS	71	7.3	10785
3l72.nb	B	/B0164-HIS	NE2	B	/B0316-TYR	OH	2.5	SS	15211.6		2503
3l72.nb	O	/O0254-HIS	ND1	O	/O0325-TYR	OH	2.5	SS	71	7.2	10712
3l73.nb	O	/O0254-HIS	ND1	O	/O0325-TYR	OH	2.5	SS	71	7.3	10623
3l74.nb	B	/B0254-HIS	ND1	B	/B0325-TYR	OH	2.5	SS	71	7.3	2858

3l75.nb	O	/O0164-HIS	NE2	O	/O0316-TYR	OH	2.5	SS	15211.7	10449
3lc3.nb	C	/C0101-HIS	ND1	C	/C0234-TYR	OH	2.5	SS	136 8.5	2327
3lcp.nb	C	/C0080-HIS	ND1	C	/C0082-TYR	OH	2.5	SS	2 5.4	2194
3lcp.nb	D	/D0080-HIS	ND1	D	/D0082-TYR	OH	2.5	SS	2 5.4	2492
3lg2.nb	A	/A0102-TYR	OH	A	/A0178-HIS	ND1	2.5	SS	7610.6	525
3li2.nb	A	/A0150-TYR	OH	A	/A0177-HIS	NE2	2.5	SS	2712.9	648
3lm7.nb	A	/A0216-HIS	ND1	A	/A0218-TYR	OH	2.5	SS	2 6.4	1743
3lma.nb	A	/A0216-HIS	NE2	A	/A0227-TYR	OH	2.5	SS	1112.0	1245
3lp9.nb	D	/D0031-TYR	OH	D	/D0181-HIS	ND1	2.5	SS	15010.0	4079
3luq.nb	C	/C0135-TYR	OH	C	/C0149-HIS	ND1	2.5	SS	1411.2	1080
3luq.nb	D	/D0135-TYR	OH	D	/D0149-HIS	ND1	2.5	SS	1411.2	1507
3m6s.nb	B	/B0022-TYR	OH	B	/B0111-HIS	ND1	2.5	SS	89 8.9	1249
3pgh.nb	B	/B0234-TYR	OH	B	/B0309-HIS	ND1	2.5	SS	7510.0	3334
3pgh.nb	C	/C0234-TYR	OH	C	/C0309-HIS	ND1	2.5	SS	75 9.9	5729
3pgh.nb	D	/D0234-TYR	OH	D	/D0309-HIS	ND1	2.5	SS	7510.0	8124
4cac.nb	A	/A0051-TYR	OH	A	/A0122-HIS	NE2	2.5	SS	7112.0	323
4cac.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.6	704
5ca2.nb	A	/A0107-HIS	NE2	A	/A0194-TYR	OH	2.5	SS	8611.7	659
5cox.nb	A	/A0133-HIS	ND1	A	/A0147-TYR	OH	2.5	SS	14 9.1	422
5cox.nb	A	/A0234-TYR	OH	A	/A0309-HIS	ND1	2.5	SS	7510.0	917
5cox.nb	B	/B0133-HIS	ND1	B	/B0147-TYR	OH	2.5	SS	14 9.1	2750
5cox.nb	C	/C0234-TYR	OH	C	/C0309-HIS	ND1	2.5	SS	7510.0	5579
5cox.nb	D	/D0234-TYR	OH	D	/D0309-HIS	ND1	2.5	SS	7510.1	7911
5tsw.nb	F	/F0015-HIS	ND1	F	/F0059-TYR	OH	2.5	SS	44 9.3	3510
6cox.nb	A	/A0234-TYR	OH	A	/A0309-HIS	ND1	2.5	SS	75 9.8	943
6cox.nb	B	/B0234-TYR	OH	B	/B0309-HIS	ND1	2.5	SS	75 9.8	3337
7gpb.nb	C	/C0571-HIS	ND1	C	/C0613-TYR	OH	2.5	SS	42 8.6	9645
9rub.nb	B	/B0286-TYR	OH	B	/B0308-HIS	NE2	2.5	SS	2211.1	3092

I. Appendix III. Tyr-Cys non-bonded contacts with TyrOH hydrogen bonds to His, Glu, or Asp.

(proteins containing metal centers within 20 Å are underlined,
protein selected for examination is in bold).

A. Histidine hydrogen bonds:

Native fungus laccase from Trametes hirsute:
pdb3fpx.nb A /A0116-TYR OH A /A0454-HIS ND1 3.1 SS 33811.2 855 /A0116-TYR CE1 A /A0205-CYS SG 3.0 SS 89 7.3 854

Crystal structure of laccase from Cerrena maxima at 1.9Å resolution:
pdb2h5u.nb A /A0116-TYR OH A /A0454-HIS ND1 3.2 SS -111.2 965 /A0116-TYR CE1 A /A0205-CYS SG 3.1 SS -1 7.5 964

Crystal structure of laccase from Cerrena maxima at 1.76Å resolution:
pdb3div.nb A /A0116-TYR OH A /A0454-HIS ND1 3.2 SS -111.2 1024 /A0116-TYR CE1 A /A0205-CYS SG 3.1 SS -1 7.5 1023

B. Aspartate or Glutamate hydrogen bonds:

Structure of E. coli AdiC (P1):
pdb3lrc.nb C /C0093-TYR OH C /C0208-GLU OE2 2.7 SS 11510.5 3870 /C0093-TYR CE1 C /C0097-CYS SG 2.7 SS 4 6.0 3869
pdb3lrc.nb A /A0093-TYR OH A /A0208-GLU OE2 2.5 SS 11510.5 481 /A0093-TYR CE1 A /A0097-CYS SG 2.8 SS 4 6.0 480
pdb3lrc.nb B /B0093-TYR OH B /B0208-GLU OE2 2.5 SS 11510.5 2175 /B0093-TYR CE1 B /B0097-CYS SG 2.8 SS 4 6.0 2174
pdb3lrc.nb D /D0093-TYR OH D /D0208-GLU OE2 2.5 SS 11510.6 5560 /D0093-TYR CE1 D /D0097-CYS SG 2.8 SS 4 6.0 5559

Crystal structure of the isocitrate lyase from Aspergillus nidulans:
pdb1dqu.nb A /A0260-ASP OD1 A /A0371-TYR OH 3.0 SS 111 8.6 1103 /A0371-TYR CE2 A /A0377-CYS SG 3.0 SS 6 9.4 1522

Crystal structure of a cupin protein (BF4112) from Bacteroides fragilis. Northeast Structural Genomics Consortium target BfR205:
pdb3cew.nb A /A0050-GLU OE1 A /A0052-TYR OH 3.1 SS 2 6.5 273 /A0052-TYR CE2 A /A0098-CYS SG 3.0 SS 46 4.8 297
pdb3cew.nb B /B0050-GLU OE1 B /B0052-TYR OH 3.1 SS 2 6.5 828 /B0052-TYR CE2 B /B0098-CYS SG 3.0 SS 46 4.8 851
pdb3cew.nb C /C0050-GLU OE1 C /C0052-TYR OH 3.1 SS 2 6.5 1395 /C0052-TYR CE2 C /C0098-CYS SG 3.0 SS 46 4.8 1418
pdb3cew.nb D /D0050-GLU OE1 D /D0052-TYR OH 3.1 SS 2 6.5 1951 /D0052-TYR CE2 D /D0098-CYS SG 3.0 SS 46 4.8 1974

Crystal structure of a TRAPP subassembly activating the Rab Ypt1p:
pdb3cue.nb K /K0061-TYR OH K /K0153-GLU OE1 3.1 SS 92 9.2 6397

/K0061-TYR CE1 K /K0065-CYS SG 3.0 SS 4 6.3 6395
pdb3cue.nb W /W0061-TYR OH W /W0153-GLU OE1 3.1 SS 92 9.2 13864 /W0061-TYR CE1 W /W0065-CYS SG 3.0 SS 4 6.3 13862

Cyclooxygenase-2 (prostaglandin synthase-2) complexed with a selective inhibitor, sc-558:
pdb1cx2.nb D /D0055-TYR OH D /D0067-GLU OE2 3.4 SS 12 9.4 7208 /D0055-TYR CE2 D /D0057-CYS SG 3.1 SS 2 7.0 7207

Crystal structure of DsbD-alpha; the N-terminal domain of DsbD:
pdb1jpe.nb A /A0042-TYR OH A /A0068-ASP OD2 2.7 SS 2611.1 243 /A0042-TYR CE2 A /A0103-CYS SG 3.1 SS 61 8.1 249

Crystal Structure of ecarpholin S complexed with suramin:
pdb3bjw.nb A /A0073-TYR OH A /A0099-ASP OD2 2.6 SS 2510.8 387 /A0073-TYR CE1 A /A0096-CYS SG 3.1 SS 22 7.1 386
pdb3bjw.nb C /C0073-TYR OH C /C0099-ASP OD2 2.7 SS 2510.7 1742 /C0073-TYR CE1 C /C0096-CYS SG 3.1 SS 22 6.9 1741
pdb3bjw.nb F /F0073-TYR OH F /F0099-ASP OD2 2.7 SS 2511.0 3631 /F0073-TYR CE1 F /F0096-CYS SG 3.1 SS 22 7.4 3630

Crystal structure of ammodytin L:
pdb3dih.nb A /A0064-TYR OH A /A0089-ASP OD2 2.6 SS 2510.9 434 /A0064-TYR CE1 A /A0086-CYS SG 3.1 SS 22 7.2 433

Crystal structure of acid-beta-glucosidase with isofagomine at neutral pH:
pdb3gxf.nb B /B0313-TYR OH B /B0340-GLU OE2 2.5 SS 27 8.7 3573 /B0313-TYR CE2 B /B0342-CYS SG 3.1 SS 29 7.7 3575

Ternary complex between trimethylamine dehydrogenase and electron transferring flavoprotein:
pdb1o95.nb A /A0110-HIS NE2 A /A0126-TYR OH 3.8 SS 16 9.6 588 /B0126-TYR CE1 B /B0136-CYS SG 2.5 SS 10 5.7 3652